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SEMI-DISCRETE SOLUTION OF A PAIR OF SIMULTANEOUS PARTIAL DIFFERENTIAL EQUATIONS

by

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled SEMI-DISCRETE SOLUTION OF A PAIR OF SIMULTANEOUS PARTIAL DIFFERENTIAL EQUATIONS submitted by S.S. LUTHRA in partial fulfilment of the requirements for the degree of Master of Science.

ABSTRACT

This thesis presents a comparative study of two procedures for generating semi-discrete solutions to the pair of simultaneous partial differential equations

$$D \frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial \theta} - K(T)C = 0$$

and

$$k \frac{\partial^2 T}{\partial x^2} - \rho C_\rho \frac{\partial T}{\partial \theta} + K(T)C = 0,$$

where C and T are functions of x and θ. These methods are based upon use of Taylor Series and Chebyshev Polynomials respectively. In both cases it is shown that the solutions so obtained are weakly stable -- ie., convergent but numerically unstable.

These partial differential equations arise in conjunction with an extended numerical treatment of the penetration theory model for the diffusion of a gas through a non-volatile liquid. The procedures investigated result in a solution interval significantly longer than that obtained by previous researchers.

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PREFACE

From the earliest attempts to predict theoretically the effect of a simultaneous chemical reaction upon the rate of gas absorption by Hatta [14], idealised models of the gas absorption process have been used extensively. This thesis employs one of the most commonly used models, namely, the penetration theory model. A pair of simultaneous partial differential equations which give concentration of gas and temperature at a known depth at a known time are derived. Two approaches to the design of computer algorithms for producing numerical solutions to these differential equations are studied in detail. The approaches are based respectively upon Taylor Series and Chebyshev Polynomials. The Taylor Series approach, although more easily handled on a formal basis, is found to possess certain inherent computational disadvantages; in this respect the solution in Chebyshev Polynomials is more efficient. For example, the former is far more prone to numerical error accumulating through numerous multiplication and division operations which are circumvented in the Chebyshev Polynomials case through the use of special matrix relations. Furthermore, "economisation" technique is not applicable to the Taylor Series approach.

Both procedures are demonstrated to be weakly stable which seriously limits the distance interval upon which the solutions

obtained remain acceptably accurate. However, both methods increase the length of the time interval for accurate solution materially beyond that of previous methods. Further extension of these intervals appears contingent upon more sophisticated approximations for the operator $\partial/\partial t$, with an attendant gross increase in mathematical complexity.

CHAPTER I

SOLUTION IN TAYLOR SERIES

1.1. Nature of the Problem

In this chapter, a set of simultaneous partial differential equations for the study of concentration of gas and temperature have been derived. The theoretical model chosen for the absorption system is deliberately simplified, and most suitable boundary conditions are adopted. The system consists of a pure gas in contact with a stagnant semi-infinite liquid phase. System parameters, such as the kinetics of the reaction, the interfacial area for mass transfer, the liquid density, viscosity and diffusivity, which are known to vary, have deliberately been taken as constants. The liquid is assumed to be non-volatile and hence the chemical reaction and temperature are assumed to vary continuously with regard to both time and distance .

1.2. Equations for Concentration and Temperature

Let an x-axis be chosen so that the absorbing fluid occupies the region $x > 0$. If $C(x,\theta)$ is the concentration of absorbed gas per unit volume at a depth x and time θ , then the rate of flow of gas across unit area perpendicular to the x-axis

is $-D \frac{\partial C}{\partial x}$ where D is the mass diffusivity. The rate of decrease of C caused by the chemical reaction is $K(T)C$ where $K(T)$ is the reaction-rate coefficient which is a function of temperature T which in turm is a function of x and θ. The mass transfer equation for the gas is, therefore,

$$\frac{\partial C}{\partial \theta} = D \frac{\partial^2 C}{\partial x^2} - K(T)C \, . \tag{1.1}$$

The concentration of gas is initially zero throughout the absorbing fluid. The concentration at the boundary at a subsequent time θ will be denoted by $f(\theta)$. Thus the concentration C must satisfy the following boundary conditions:

$$C(0,\theta) = f(\theta) \, , \tag{1.2a}$$

$$C(x,0) = 0 \, , \tag{1.2b}$$

$$C(\infty,\theta) = 0. \tag{1.2c}$$

The chemical reaction which decreases C at the rate $K(T)C$ absorbs heat at the rate $\Delta K(T)C$, where Δ is measured in BTU per lb. mole. However, any temperature change involves a rate of increase of heat of the amount $\rho C_\rho \cdot \frac{\partial T}{\partial \theta}$ where ρ is the molal density and C_ρ is the molal specific heat. If the thermal conductivity is k, the heat transfer equation is

(1.3) $$k \frac{\partial^2 T}{\partial x^2} = \rho C_\rho \frac{\partial T}{\partial \theta} - \Delta K(T)C ,$$

which may be written in the form

(1.4) $$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T}{\partial \theta} + \frac{1}{\alpha_1}\left(\frac{\Delta}{\rho C_\rho}\right)K(T)C = 0 ,$$

where $\alpha_1 = k/\rho C_\rho$ is the thermal diffusivity.

If T_o denotes the constant temperature throughout the liquid at time $\theta = 0$ and $g(\theta)$ the temperature at the boundary at subsequent time θ, then the boundary conditions satisfied by T are as follows:

(1.5a) $$T(0,\theta) = g(\theta) ,$$

(1.5b) $$T(x,0) = T_o ,$$

(1.5c) $$T(\infty,\theta) = T_o .$$

Equations (1.1) and (1.4) form a pair of simultaneous partial differential equations for determination of $C(x,\theta)$ and $T(x,\theta)$. In the special instance that the reaction-rate coefficient is a constant K_o, the single equation (1.1) serves to determine $C(x,\theta)$. Substitution of the solution $C(x,\theta)$ into the equation (1.4) provides a single equation for the determination of the

temperature $T(x,\theta)$.

1.3. Danckwerts Solution for Constant Reaction Rate and Constant Boundary Conditions

Danckwerts[5] solved equation (1.1) with $K(T) = K_o$ and with constant $f(\theta) = C_c$. His solution involves the complement of the error function and is as follows:

$$C = \frac{1}{2} C_c \exp[-(K_o/D)^{\frac{1}{2}}x] \operatorname{erfc}[\frac{x}{2(D\theta)^{\frac{1}{2}}} - (K_o\theta)^{\frac{1}{2}}]$$

$$+ \frac{1}{2} C_c \exp[(K_o/D)^{\frac{1}{2}}x] \operatorname{erfc}[\frac{x}{2(D\theta)^{\frac{1}{2}}} + (K_o\theta)^{\frac{1}{2}}] \,. \tag{1.6}$$

For unit area of the surface at $x = 0$, the rate of absorption of the gas is $-D \frac{\partial C}{\partial x}$ and it follows from (1.6) that this rate is

$$C_c(DK_o)^{\frac{1}{2}}[\operatorname{erfc}(K_o\theta)^{\frac{1}{2}} + (\pi K_o\theta)^{-\frac{1}{2}}\exp(-K_o\theta)] \,. \tag{1.7}$$

In the absence of any chemical reaction, the term $K(T)C$ is omitted from equation (1.1) and the rate $-D \frac{\partial C}{\partial x}$ is equal to

$$C_c(D/\pi\theta)^{\frac{1}{2}} \,. \tag{1.8}$$

The ratio of the expressions (1.7) and (1.8) is equal to

$$\phi_1(\theta) = (\pi K_o\theta)^{\frac{1}{2}}\text{erf}(K_o\theta)^{\frac{1}{2}} + \exp(-K_o\theta) \ . \tag{1.9}$$

At time $\theta = 0$ the value of $\phi_1(\theta)$ is unity. At any subsequent time θ, the value of $\phi_1(\theta)$ indicates the factor by which the rate of absorption of gas has increased during this time interval due to the chemical reaction.

1.4. Effect of Linear Boundary Condition

The boundary condition of constant $f(\theta)$ is clearly unrealistic if the overall temperature of the system increases as the reaction proceeds. Sullivan [22] has treated boundary conditions (1.2a) and (1.5a) of the form

$$C(0,\theta) = a_1 + a_2T(0,\theta) \ , \tag{1.10a}$$

$$T(0,\theta) = T_o + a\theta \ , \tag{1.10b}$$

where a, a_1, a_2 and T_o are constants. However, he has taken $K(T)$ to be a constant K_o. Under these circumstances, he derived the following formulas for $C(x,\theta)$ and $T(x,\theta)$:

$$(1.11a)\qquad C(x,\theta) = (a_1+a_2T_o)\int_o^\theta H_d(x,\theta)\exp(-K_o\theta)d\theta$$

$$+ aa_2\int_o^\theta d\theta\int_o^\theta H_d\exp(-K_o\theta)d\theta,$$

$$(1.11b)\qquad T(x,\theta) = T_o + a\int_o^\theta d\theta\int_o^\theta H_a(x,\theta)d\theta$$

$$-\frac{\Delta K_o}{\rho C_\rho}(a_1+a_2T_o)\int_o^\theta d\theta\,\frac{\exp(-n\theta)}{(\alpha_1/D)-1}\int_o^\theta [H_d(x,\theta)\exp(Dn\theta/\alpha_1)$$

$$-H_a(x,\theta)\exp(n\theta)]d\theta$$

$$-\frac{\Delta K_o}{\rho C_\rho}aa_2\int_o^\theta d\theta\int_o^\theta d\theta\,\frac{\exp(-n\theta)}{(\alpha_1/D)-1}\int_o^\theta [H_d\exp(Dn\theta/\alpha_1)$$

$$-H_a\exp(n\theta)]d\theta\ ,$$

where the functions $H_d(x,\theta)$, $H_a(x,\theta)$ and constant n are defined as follows:

$$(1.12a)\qquad H_d(x,\theta) = \frac{x}{2(\pi D\theta^3)^{\frac{1}{2}}}\exp(-x^2/4D\theta)\ ,$$

$$(1.12b)\qquad H_a(x,\theta) = \frac{x}{2(\pi\alpha_1\theta^3)^{\frac{1}{2}}}\exp(-x^2/4\alpha_1\theta)\ ,$$

$$(1.12c)\qquad n = \frac{\alpha_1K_o}{\alpha_1-D}\ .$$

The equations (1.11) were integrated numerically by Sullivan [22] who then computed $\partial C/\partial x$ at $x = 0$ by the following approximation where x_1 is a small number.

$$(1.13) \qquad \left(\frac{\partial C}{\partial x}\right)_{x=o} = \frac{-3C(0,\theta)+4C(x_1,\theta)-C(2x_1,\theta)}{2x_1} .$$

Values of the ratio $\phi_2(\theta)$ which corresponds to $\phi_1(\theta)$ under the changed conditions, were found from

$$(1.14) \qquad \phi_2(\theta) = \frac{-D(\partial C/\partial x)_{x=o}}{C(0,\theta)(D/\pi\theta)^{\frac{1}{2}}} ,$$

and were plotted as functions of $M = (\pi K_o \theta)^{\frac{1}{2}}$. The values of parameters were chosen to correspond to several physical situations in which CO_2 at a pressure of one atmosphere is absorbed into 1M NaOH.

The ratio $\phi_1(\theta)$ was derived under the assumption of a constant reaction-rate $K(T) = K_o$ and a constant surface concentration $C(0,\theta) = C_c$. The ratio $\phi_2(\theta)$ was derived under the assumption that $K(T) = K_o$ and that the surface concentration and temperature are both linear functions of time. The study of $C(x,\theta)$ and $T(x,\theta)$ when $K(T)$ is not constant is the subject of the following sections and the subsequent chapters.

1.5. Characteristics of the Two Partial Differential Equations

To a large extent, the strategy to be adopted for the solution of a partial differential equation depends upon the nature of the equation, although the initial and boundary conditions play very prominent roles. In this section, a study of the characteristics of the equations (1.1) and (1.4) is made and domains of solution obtained.

Consider the diffusion equation (1.1), namely

$$D \frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial \theta} + K(T)C \,, \tag{1.15}$$

where C, $\partial C/\partial x$ and $\partial C/\partial \theta$ are given on a curve π in the $x - \theta$ plane. Since $C = C(x,\theta)$, we may write

$$dC = \frac{\partial C}{\partial x} dx + \frac{\partial C}{\partial \theta} d\theta \,, \tag{1.16a}$$

$$d \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2} dx + \frac{\partial^2 C}{\partial x \partial \theta} d\theta \,, \tag{1.16b}$$

$$d \frac{\partial C}{\partial \theta} = \frac{\partial^2 C}{\partial x \partial \theta} dx + \frac{\partial^2 C}{\partial \theta^2} d\theta \,. \tag{1.16c}$$

The equations (1.15), (1.16b) and (1.16c) lead to

[illegible]

[illegible]

$$[illegible]$$

[illegible]

$$[illegible]$$

$$[illegible]$$

$$[illegible]$$

[illegible]

$$(1.17)\qquad \begin{bmatrix} dx & d\theta & 0 \\ 0 & dx & d\theta \\ D & 0 & 0 \end{bmatrix} \begin{bmatrix} \dfrac{\partial^2 C}{\partial x^2} \\ \dfrac{\partial^2 C}{\partial x \partial \theta} \\ \dfrac{\partial^2 C}{\partial \theta^2} \end{bmatrix} = \begin{bmatrix} d(\dfrac{\partial C}{\partial x}) \\ d(\dfrac{\partial C}{\partial \theta}) \\ \dfrac{\partial C}{\partial \theta} + K(T)C \end{bmatrix} .$$

If

$$(1.18)\qquad \begin{vmatrix} dx & d\theta & 0 \\ 0 & dx & d\theta \\ D & 0 & 0 \end{vmatrix} = D(d\theta)^2 \neq 0 ,$$

the values of $\dfrac{\partial^2 C}{\partial x^2}$, $\dfrac{\partial^2 C}{\partial x \partial \theta}$ and $\dfrac{\partial^2 C}{\partial \theta^2}$ may be determined uniquely. Hence the characteristic equations in the $x - \theta$ plane, beneath which the solution is valid, are determined by

$$(1.19)\qquad D(d\theta)^2 = 0 ,$$

which gives two coincident characteristics, namely, the lines

$$\theta = \text{constant},$$

and hence the equation is parabolic. These lines run from $x = 0$ to $x = \infty$. Hence the required region of the $x - \theta$ plane is enclosed by characteristics and, therefore, our solutions are valid.

Similar remarks apply to the temperature equation (1.4), namely,

$$\alpha_1 \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial \theta} - \frac{\Delta}{\rho C_\rho} K(T)C \;, \tag{1.20}$$

and, therefore, we can proceed with the solution of both the equations.

1.6. Treatment of Linear Reaction Rate and General Boundary Conditions

The function $K(T)$ is a continuous function of T. Provided the temperature changes are small, it may be approximated by putting

$$K(T) = \ell + mT \;, \tag{1.21}$$

where ℓ and m are suitably chosen constants. It will hereafter be supposed that the temperature T is measured as the excess of temperature above the constant temperature at time $\theta = 0$. Thus $T_o = 0$ and equations (1.1) and (1.4) may be expressed in the form

$$\frac{\partial^2 C}{\partial x^2} - \frac{1}{D}\frac{\partial C}{\partial \theta} - (L+MT)C = 0 \;, \tag{1.22a}$$

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T}{\partial \theta} + \sigma(L+MT)C = 0 \;, \tag{1.22b}$$

where

(1.23) $L = \ell/D$, $M = m/D$, $\sigma = (1/\alpha_1)(\Delta/\rho C_\rho)D = \Delta D/k$.

With $K(T)$ chosen as in (1.21), the solutions $C(x,\theta)$ and $T(x,\theta)$ of equations (1.22) are also functions of M and they may be expanded as infinite series of the type

(1.24a) $$C(x,\theta) = \sum C_s(x,\theta)M^s ,$$

(1.24b) $$T(x,\theta) = \sum T_s(x,\theta)M^s ,$$

where the summations are in s from zero to infinity.

Substitution of the expansions (1.24) into (1.22), and comparison of the terms that involve equal powers of M, leads to successive pairs of equations for the determination of the functions $C_s(x,\theta)$ and $T_s(x,\theta)$ which in turn are successive terms in approximations to $C(x,\theta)$ and $T(x,\theta)$ respectively. For example, the terms independent of M lead to the equations

(1.25a) $$\frac{\partial^2 C_o}{\partial x^2} - \frac{1}{D}\frac{\partial C_o}{\partial \theta} - LC_o = 0 ,$$

(1.25b) $$\frac{\partial^2 T_o}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T_o}{\partial \theta} + \sigma LC_o = 0 ,$$

and the terms that involve M lead to the equations

(1.26a) $$\frac{\partial^2 C_1}{\partial x^2} - \frac{1}{D}\frac{\partial C_1}{\partial \theta} - LC_1 = T_o C_o ,$$

(1.26b) $$\frac{\partial^2 T_1}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T_1}{\partial \theta} + \sigma LC_1 = -\sigma T_o C_o .$$

In general

(1.27a) $$\frac{\partial^2 C_i}{\partial x^2} - \frac{1}{D}\frac{\partial C_i}{\partial \theta} - LC_i = \sum_{j=o}^{i-1} T_j C_{i-1-j} ,$$

(1.27b) $$\frac{\partial^2 T_i}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T_i}{\partial \theta} + \sigma LC_i = -\sigma \sum_{j=o}^{i-1} T_j C_{i-1-j} ,$$

where $i = 1,2,3,\ldots$.

For the linear boundary conditions (1.10), the expressions (1.11) are solutions of equations (1.25) but they are not suitable for substitution in the differential equation (1.26). In the following section, the solution of equations (1.25) is obtained in a more convenient form.

1.7. Semi-Discrete Solution for $C_o(x,\theta)$ and $T_o(x,\theta)$

In a manner similar to that of section 1.5 it can be seen that the partial differential equations (1.25), (1.26) and (1.27) are of the parabolic type with characteristics which satisfy the equation θ = constant. Hence a valid solution may be obtained for $x \geq 0$, $\theta \geq 0$. We therefore rewrite the above

equations by putting

$$\text{(1.28)} \qquad \theta_r = r\Delta\theta, \quad C_o(x,\theta_r) = C_o^{(r)}(x), \quad T_o(x,\theta_r) = T_o^{(r)}(x) \ ,$$

and using the following approximations where r ranges from zero to infinity:

$$\text{(1.29a)} \qquad \left[\frac{\partial C_o(x,\theta)}{\partial\theta}\right]_{r+1} = \frac{C_o^{(r+1)}(x)-C_o^{(r)}(x)}{\Delta\theta} \ ,$$

$$\text{(1.29b)} \qquad \left[\frac{\partial T_o(x,\theta)}{\partial\theta}\right]_{r+1} = \frac{T_o^{(r+1)}(x)-T_o^{(r)}(x)}{\Delta\theta} \ .$$

Equations (1.25) are then equivalent to the following set of ordinary differential equations valid for each value of $r \geq 0$.

$$\text{(1.30a)} \qquad \frac{d^2C_o^{(r+1)}}{dx^2} - \alpha C_o^{(r+1)} = -\beta C_o^{(r)},$$

$$\text{(1.30b)} \qquad \frac{d^2T_o^{(r+1)}}{dx^2} - \gamma T_o^{(r+1)} = -\gamma T_o^{(r)} - \lambda C_o^{(r+1)},$$

where $\alpha,\beta,\gamma,\lambda$ denote the positive quantities

$$\text{(1.31a)} \qquad \alpha = \frac{1}{D\Delta\theta} + L \ , \qquad \beta = \frac{1}{D\Delta\theta} \ ,$$

$$\text{(1.31b)} \qquad \gamma = \frac{1}{\alpha_1\Delta\theta} \ , \qquad \lambda = \sigma L \ .$$

Let f_r and g_r denote $f(\theta_r)$ and $g(\theta_r)$. The boundary conditions for $C_o^{(r)}$ and $T_o^{(r)}$ are then

$$(1.32a) \qquad C_o^{(r)}(x=0) = f_r , \quad T_o^{(r)}(x=0) = g_r, \quad (r > 0)$$

$$(1.32b) \qquad C_o^{(0)}(x) = 0 , \qquad T_o^{(0)}(x) = 0 ,$$

$$(1.32c) \qquad C_o^{(r)}(x=\infty) = 0 . \quad T_o^{(r)}(x=\infty) = 0 .$$

For $r = 0$ and 1, the equations (1.30) and (1.32) determine $C_o^{(1)}(x)$ and $C_o^{(2)}(x)$ as

$$C_o^{(1)}(x) = f_1 \exp(-\alpha^{\frac{1}{2}}x) ,$$

$$C_o^{(2)}(x) = \exp(-\alpha^{\frac{1}{2}}x)[f_2 + \frac{\beta f_1}{2\alpha^{\frac{1}{2}}} x] .$$

For general values of r, the solution of (1.30a) has the form

$$(1.33) \qquad C_o^{(r)}(x) = \exp(-\alpha^{\frac{1}{2}}x) \sum_{n=o}^{r-1} B_{rn} x^n ,$$

and if this expression is substituted into (1.30a), there result the equations

$$(1.34a) \qquad B_{r+1,n} = \frac{\beta}{2n\alpha^{\frac{1}{2}}} B_{r,n-1} + \frac{n+1}{2\alpha^{\frac{1}{2}}} B_{r+1,n+1} ,$$

$$n = 1(1)r, \quad B_{r,s} = 0 \quad \text{for} \quad s \geq r,$$

(1.34b) $$B_{r,o} = f_r \ .$$

These recurrence relations may be used to provide the values of $B_{r,n}$ in reverse order, starting from $B_{1,o} = f_1$. Equations (1.34a) determine $B_{r,n}$ at points of a net in which the points of co-ordinates $(r+1,r)$ and $(r,0)$ form boundaries on which the values of $B_{r,n}$ are known by virtue of (1.34b) and a similar previous use of (1.34a). The $B_{r,n}$ at internal nodes of the net may be determined by steps along lines of constant r values. In contrast, if equation (1.25a) were integrated directly by the use of a difference net in the x,θ plane, then the boundary conditions on x involve two boundaries $x = 0$ and $x = \infty$. However, in the technique adopted by us, the inclusion of the exponential factor in expression (1.33) ensures that the boundary condition at $x = \infty$ is satisfied and it results in a simplified difference net for the $B_{r,n}$.

For the special case in which $K(T) = K_o$, $C_o(x,\theta)$ coincides with $C(x,\theta)$ and the ratio $\phi(\theta)$ analogous to (1.9) or (1.14) is given by

(1.35) $$\phi^{(0)}(\theta_r) = (\pi D\theta_r)^{\frac{1}{2}}(\alpha^{\frac{1}{2}} - \frac{B_{r,1}}{f_r}) \ .$$

It may be remarked in passing that the recurrence relations (1.34) are significantly more convenient for numerical computation than the integral expressions (1.11). The recurrence

formulas are well-behaved in the sense that they may be repeated several thousand times without introduction of serious round-off errors.

The co-efficients $B_{r,n}$ given by the relations (1.34) determine the function $C_o^{(r)}(x)$ and hence the concentration $C_o(x,\theta)$ at times $\theta = r\Delta\theta$ at depth x.

In a similar manner, the temperature $T_o(x,\theta)$ may be obtained from equation (1.30b). For $r = 0$, it has for solution

$$(1.36) \qquad T_o^{(1)}(x) = (g_1 + \frac{\lambda f_1}{\alpha-\gamma}) \exp(-\gamma^{\frac{1}{2}}x) - \frac{\lambda f_1}{\alpha-\gamma} \exp(-\alpha^{\frac{1}{2}}x) .$$

For general values of r, the solution $T_o^{(r)}(x)$ may be expressed in the form

$$(1.37) \qquad T_o^{(r)}(x) = L_r \exp(-\gamma^{\frac{1}{2}}x) \sum_{n=o}^{r-1} G_{rn}x^n + M_r \exp(-\alpha^{\frac{1}{2}}x) \sum_{n=o}^{r-1} H_{rn}x^n ,$$

in which the introduction of the normalising constants L_r and M_r allows the stipulation that

$$(1.38) \qquad G_{r,r-1} = M_{r,r-1} = 1 .$$

The second of the conditions (1.32a) implies that

$$(1.39) \qquad L_r G_{ro} + M_r H_{ro} = g_r .$$

Substitution of the expressions (1.33) and (1.37) into the equation (1.30b), and the use of relation $G_{r,r-1} = 1$, leads to the equation

$$L_{r+1} = \frac{\gamma^{\frac{1}{2}} L_r}{2r} , \tag{1.40}$$

and to the following recurrence relations involving the G_{rn} .

$$G_{r+1,r} = 1 , \tag{1.41a}$$

$$G_{r+1,n} = \frac{r}{n} G_{r,n-1} + \frac{n+1}{2\gamma^{\frac{1}{2}}} G_{r+1,n+1}, \quad n = 1(1)r - 1, \tag{1.41b}$$

$$G_{r+1,o} = \text{indeterminate except when } r = 0. \tag{1.41c}$$

These equations determine all the coefficients G_{rn} except those of the type G_{ro} . The substitution also leads to the equation

$$M_r = \frac{-\lambda B_{r,r-1}}{\alpha-\gamma} , \tag{1.42}$$

and to the following recurrence relations involving the H_{rn}.

$$\begin{aligned} H_{r+1,n} = {} & \frac{2(n+1)\sqrt{\alpha}}{\alpha-\gamma} H_{r+1,n+1} - \frac{(n+1)(n+2)}{\alpha-\gamma} H_{r+1,n+2} \\ & - \frac{2\gamma\alpha^{\frac{1}{2}} r}{\beta(\alpha-\gamma)} H_{r,n} + \frac{B_{r+1,n}}{B_{r+1,r}} , \end{aligned} \tag{1.43a}$$

for $n = 0(1)r - 1$, with $H_{rs} = 0$ for $s \geq r$,

These recurrence relations determine all $H_{r,n}$ in the reverse order in terms of the $B_{r,n}$ starting with the known $H_{10} = 1$.

To sum up, for each value of $r \geq 0$, the relations (1.34) may be used to determine the $H_{r+1,n}$; equations (1.43) may be used to determine the $M_{r+1,n}$; and the equations (1.41) may be used to determine the $G_{r+1,n}$ except for $G_{r+1,o}$. Equations (1.40), (1.42) and (1.39) then serve to determine L_{r+1}, M_{r+1} and $G_{r+1,o}$ respectively. Initial values corresponding to $r = 0$ are

(1.44a) $$B_{10} = f_1 ,$$

(1.44b) $$G_{10} = 1 ,$$

(1.44c) $$H_{10} = 1 ,$$

(1.44d) $$L_1 = g_1 + \frac{\lambda f_1}{\alpha-\gamma} ,$$

(1.44e) $$M_1 = \frac{-\lambda f_1}{\alpha - \gamma} .$$

1.8. Semi-Discrete Solution for $C_1(x,\theta)$

The semi-discrete method may be used to solve the equations (1.26) for $C_1(x,\theta_r) = C_1^{(r)}(x)$ and $T_1(x,\theta_r) = T_1^{(r)}(x)$. Representation of the derivatives as in relations (1.29) and substitution into the equation (1.26a) leads to the following ordinary differential equation for the determination of $C_1^{(r)}(x)$.

(1.45) $$\frac{d^2C_1^{(r+1)}}{dx^2} - \alpha C_1^{(r+1)} = -\beta C_1^{(r)} + C_o^{(r+1)} T_o^{(r+1)} .$$

In view of the known expressions for $C_o^{(r+1)}$ and $T_o^{(r+1)}$, the above equation may be written as

(1.46) $$\frac{d^2C_1^{(r+1)}}{dx^2} - \alpha C_1^{(r+1)} = -\beta C_1^{(r)} + L_{r+1} \exp(-\nu x) \sum_{n=o}^{2r} P_{r+1,n} x^n$$

$$+ M_{r+1} \exp(-2\alpha^{\frac{1}{2}} x) \sum_{n=o}^{2r} Q_{r+1,n} x^n ,$$

where $P_{r+1,n}$, $Q_{r+1,n}$ and ν are the known constants determined by the equations (in which $0 \leq n \leq 2r - 2$)

(1.47a) $$P_{rn} = \sum_{s=o}^{n} B_{r,n-s} G_{rs} ,$$

(1.47b) $$Q_{rn} = \sum_{s=o}^{n} B_{r,n-s} H_{rs} ,$$

(1.47c) $$\nu = \gamma^{\frac{1}{2}} + \alpha^{\frac{1}{2}} .$$

Since the functions $C_o^{(r)}(x)$ were chosen to satisfy the boundary conditions (1.32), the corresponding conditions on $C_1^{(r)}(x)$ are zero conditions.

When $r = 0$, the solution $C_1^{(1)}(x)$ of equation (1.46) is as follows:

$$(1.48) \quad C_1^{(1)}(x) = \frac{L_1P_{10}}{\nu^2-\alpha}\,[\exp(-\nu x)-\exp(-\alpha^{\frac{1}{2}}x)] + \frac{M_1Q_{10}}{3\alpha}\,[\exp(-2\alpha^{\frac{1}{2}}x)-\exp(-\alpha^{\frac{1}{2}}x)] \ .$$

For general values of r, the solution may be expressed in the form

$$(1.49) \qquad C_1^{(r)}(x) = \exp(-\alpha^{\frac{1}{2}}x)\sum_{n=o}^{r-1} U_{rn}x^n + \exp(-\nu x)\sum_{n=o}^{2r-2} V_{rn}x^n$$
$$+ \exp(-2\alpha^{\frac{1}{2}}x)\sum_{n=o}^{2r-2} W_{rn}x^n \ ,$$

and the zero conditions on the boundary imply that for all r

$$(1.50) \qquad U_{ro} = -V_{ro} - W_{ro} \ .$$

Substitution of the expression (1.49) into (1.46) leads to the following equations for determination of the V_{rn} in terms of the known constants L_r, M_r, P_{rn} :

$$(1.51) \qquad V_{r+1,n} = \frac{2\nu(n+1)}{\nu^2-\alpha}\,V_{r+1,n+1} - \frac{(n+1)(n+2)}{\nu^2-\alpha}\,V_{r+1,n+2}$$

$$- \frac{\beta V_{rn}}{\nu^2-\alpha} + \frac{L_{r+1}P_{r+1,n}}{\nu^2-\alpha} ,$$

for $n = 0(1)2r$, with $V_{rs} = 0$ for $s \geq 2r - 1$.

The corresponding equations for determination of the W_{rn} are obtained from (1.51) by substitution of M_{r+1} for L_{r+1}, $Q_{r+1,n}$ for $P_{r+1,n}$, and $2\alpha^{\frac{1}{2}}$ for ν.

The equations for determination of the U_{rn} are identical to the equations (1.34a) in which each B_{rn} is replaced by U_{rn}; the U_{ro} are determined from the relations (1.50) instead of (1.34b). In particular the value of U_{10} is

(1.52) $$U_{10} = - \frac{L_1P_{10}}{\nu^2-\alpha} - \frac{M_1Q_{10}}{3\alpha} ,$$

$$= - V_{10} - W_{10} .$$

The ratio corresponding to (1.35) is $\phi^{(0)}(\theta_r) + M\phi^{(1)}(\theta_r)$ where

(1.53) $$\phi^{(1)}(\theta_r) = \frac{(\pi D\theta_r)^{\frac{1}{2}}}{f_r} (\alpha^{\frac{1}{2}}W_{ro}+\gamma^{\frac{1}{2}}V_{ro}-U_{r1}-V_{r1}-W_{r1}) .$$

The next, and the improved, approximation to $C(x,\theta)$ is $C_o(x,\theta) + MC_1(x,\theta)$.

CHAPTER II

SOLUTION IN CHEBYSHEV SERIES

2.1. Typical Characteristics of the Solution

In this chapter, it is proposed to consider the solution of the simultaneous partial differential equations (1.1) and (1.4) in terms of Chebyshev series.

The reduced system (1.30) and (1.45) suggests that inherent instability exists in this case. The Complementary Function of the differential equation (1.30a), namely,

$$\frac{d^2C_o^{(r+1)}}{dx^2} - \alpha C_o^{(r+1)} = -\beta C_o^{(r)} , \quad \alpha > 0, \tag{2.1}$$

is of the form

$$C_o^{(r+1)} = Ae^{\sqrt{\alpha}x} + Be^{-\sqrt{\alpha}\,x} . \tag{2.2}$$

However, the boundary conditions for $x = \infty$ force it to the form

$$C_o^{(r+1)} = Be^{-\sqrt{\alpha}\,x} , \tag{2.3}$$

eliminating the term $Ae^{\sqrt{\alpha}\,x}$ which, in fact, is a major contributor

towards $C_o^{(r+1)}$ for large values of x. Any approximation technique introduces this factor into the complementary solution in the form of round-off error. Thus the calculated solution may increase asymptotically in comparison with the true solution. In Chapter IV, the problem has been considered in some detail and it is proved that if stability can be achieved, the solution is convergent. The problem of stability does not arise if there are no round-off and truncation errors. But this is very difficult to ensure for a computed solution. If a small error is introduced in moving from point A to point B on the curve ψ (Fig 2.1) which represents true solution, so that the computed point is C, even if no error is introduced thereafter, the computed solution, for large interval, can lead to N -- a result enormously different from the true solution. Even for small intervals, the final solution may be sufficiently removed from the true solution so as to make it completely useless for all practical purposes.

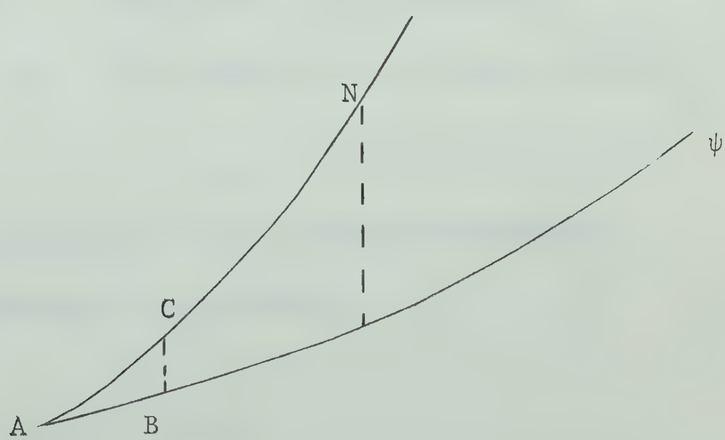

Fig. 2.1. Propagation of error.

The only way to meet such a contingency is to keep the increments in independent variables small. But in general this is also not a very satisfactory technique. It will be far more useful to maneuver the error into ripple-like character so that any divergence introduced at any step is negated immediately afterwards. Moreover, the fastest rate of convergence should be the target so as to meet the delicate situation. It is with these factors in mind that the solution of differential equations (1.30) and (1.45) have been represented in terms of Chebyshev Series.

2.2. Chebyshev Polynomials

The Chebyshev Polynomials belong to the general class of functions, the Ultraspherical Polynomials $P_n^{(\alpha)}(x)$ defined as

$$P_n^{(\alpha)}(x) = C_n(1-x^2)^{-\alpha} \frac{d^n}{dx^n}(1-x^2)^{n+\alpha}, \quad (-1 \leq \alpha < \infty), \tag{2.4a}$$

where C_n is a constant and n the degree of the polynomial. They are orthogonal over $[-1,1]$ with respect to the weight function $w(x) = (1-x^2)^{\alpha}$.

For $\alpha = 0$, they correspond to the Legendre Polynomials which are alternatively defined by the relation

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2-1)^n, \tag{2.4b}$$

and satisfy the recurrence relation

(2.5) $$P_{n+1}(x) = \frac{2n+1}{n+1} xP_n(x) - (\frac{n}{n+1})P_{n-1}(x) ,$$

and the orthogonality relation

(2.6) $$\int_{-1}^{1} P_m(x)P_n(x)dx = \frac{2}{2n+1} \quad (m = n) ,$$

$$= 0 \quad (m \neq n) .$$

An interesting property of the Legendre Polynomials concerning least square norm is stated in the theorem following the

Definition 2.1. *The Least Square Norm of a function* $f(x)$ *with weight function* $w(x)$ *over an interval* $[a,b]$ *is defined as*

$$||f(x)|| = \int_a^b w(x)f^2(x)dx .$$

Theorem 2.1. *Of all the monic polynomials (i.e. with the coefficient of* x^n *unity) defined over the interval* $[-1,1]$, *the Legendre polynomial* $C_nP_n(x)$ *where* C_n *is chosen to make the coefficient of* x^n *unity, have the least square norm, with the weight function unity.*

The proof of the above may be obtained from any standard text. (See, for example, Synder [23]).

Another important property of all orthogonal polynomials, and very useful in the context of the problem, is stated as

Theorem 2.2. *If the weight function* $w(x)$ *does not change sign in the interval* $[a,b]$*, the polynomial* $\pi_n(x)$ *which is a member of an orthogonal set of polynomials, possesses* n *distinct real zeroes all of which lie in the same interval* $[a,b]$.

For proof, see Synder [23].

The above theorem guarantees that $P_n(x)$ has n real and distinct zeroes in $[-1,1]$. Thus $P_n(x)$ oscillates around zero with variable amplitude which increases as we move towards the end points. This corresponds to the case $-\frac{1}{2} < \alpha < \infty$. However, for $-1 \leq \alpha < -\frac{1}{2}$, the amplitude of the oscillations decreases as we move from the origin towards the end points of the same interval. For $\alpha = -\frac{1}{2}$, the amplitude remains constant and the polynomials that correspond to this case are called Chebyshev Polynomials denoted by $T_n(x)$. The corresponding weight function is

$$w(x) = (1-x^2)^{-\frac{1}{2}} , \tag{2.8}$$

which serves to keep the error small near the ends of the range.

Thus Chebyshev Polynomials form an orthogonal set with respect to the weight function (2.8). Also they have all the zeros real, distinct, and lying in the interval $[-1,1]$. They oscillate around zero with constant amplitude unity throughout the interval $[-1,1]$. This is sometimes referred to as the "equal ripple property".

A few standard results for Chebyshev Polynomials have been recorded without proof in Appendix A. The following definitions and theorems are necessary here.

Definition 2.2. *The norm of the function $f(x)$ in the interval $[a,b]$ is defined as*

$$(2.9) \qquad \|f(x)\| = \sup_{a \leq x \leq b} |f(x)| .$$

Theorem 2.3. *Of all the monic polynomials of degree n on the interval $[-1,1]$, the polynomial $2^{1-n}T_n(x)$ has the smallest norm in the above sense and that*

$$(2.10) \qquad \|2^{1-n}T_n(x)\| = 2^{1-n} .$$

Synder [23] has proved it and stated it in a more useful form as:

Among all the polynomials of degree n, with maximum

norm unity in the interval $[-1,1]$, $T_n(x)$ *has the largest leading coefficient, namely,* 2^{1-n}.

This immediately leads to the

Theorem 2.4. *In the class of Ultraspherical Polynomials, Chebyshev Polynomials yield expansions which display the strongest possible convergence.*

For proof, see Synder [23]. He has further proved that the Taylor Series which is a limiting case of Ultraspherical Polynomails for $\alpha = \infty$ display the worst possible convergence.

2.3. Truncation Error

If a function $f(x)$ is expanded in terms of Ultraspherical Polynomials, that is

$$f(x) = \sum_{N=o}^{n} C_N P_N^{(\alpha)}(x) \ , \tag{2.11}$$

and is approximated by

$$f^*(x) = \sum_{N=o}^{n-1} C_N P_N^{(\alpha)}(x) \ , \tag{2.12}$$

the truncation error is

(2.13) $$\varepsilon_n(x) = C_n P_n^{(\alpha)}(x) \ .$$

For Taylor Series, $\alpha = \infty$ and $\varepsilon_n(x) = C_n x^n$ which increases continuously as we move from the origin towards the end points. For Legendre Polynomials, $\alpha = 0$ and $\varepsilon_n(x) = C_n P_n(x)$ which is lowest at the origin but increases as we move towards the end points ± 1 and is of maximum magnitude C_n. For Chebyshev Series, $\alpha = -\frac{1}{2}$ and $\varepsilon_n(x) = C_n T_n(x)$ which has an equal ripple cosine curve. (Fig. 2.2). Thus error is more evenly distributed over the entire range.

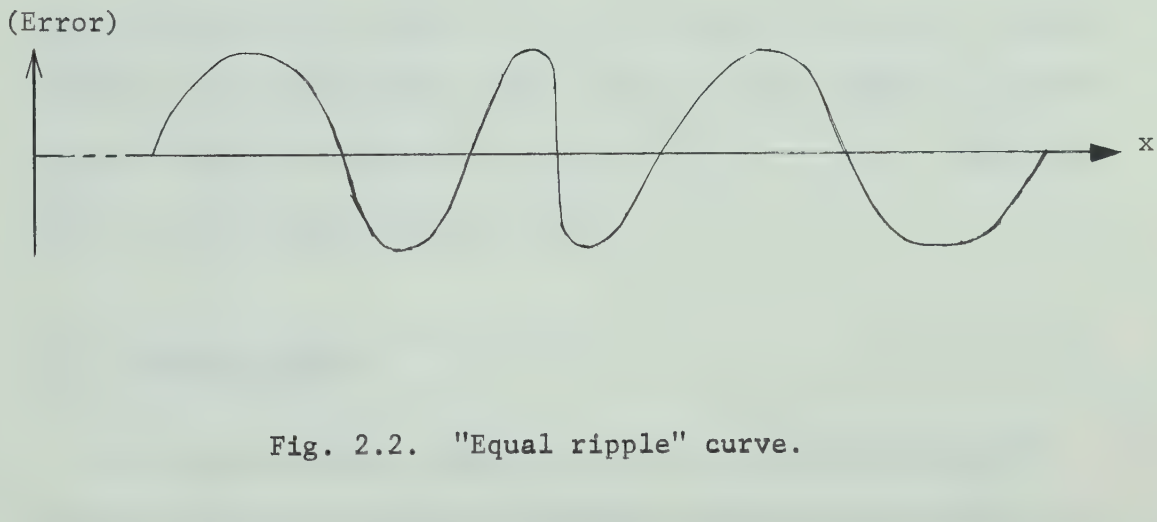

Fig. 2.2. "Equal ripple" curve.

A Taylor Series expansion of a function will have large coefficients even though the size of the function throughout the range may be small whereas the Chebyshev form will have much smaller coefficients and hence a greater facility for significant

truncation with little error.

Any finite range $[a,b]$ may be linearly transformed to $[-1,1]$ to which pertain the Chebyshev Polynomials. Similarly to the range $[0,1]$ pertain the (shifted) Chebyshev Polynomials, defined as

$$(2.14) \qquad T_n^*(x) = T_n(2x-1) = 2T_n^2(\sqrt{x}) - 1 = T_{2n}(\sqrt{x}) \ , \quad 0 \leq x \leq 1 \ ,$$

with corresponding weight function

$$(2.15) \qquad w(x) = [1-(2x-1)^2]^{-\frac{1}{2}} = [4x(1-x)]^{-\frac{1}{2}} \ .$$

It is interesting to note that for the approximation of a general function $f(x)$, we should expect, with the same number of terms, to get a smaller minimax error with $T_r^*(x)$ in $[0,1]$ than with $T_r(x)$ in the larger range $[-1,1]$.

2.4. Fourier Series

Since Fourier Series are based on use of orthogonal functions and are intimately connected with Chebyshev Series, in this section, it is proposed to consider the same and compare the convergence properties of the two.

The trigonometric functions $1, \cos x, \cos 2x, \ldots, \sin x, \sin 2x, \ldots$ are orthogonal with respect to the weight function

unity in the interval $[-\pi,\pi]$. Hence the trigonometric polynomial

$$(2.16) \qquad p_n(x) = \frac{1}{2} a_o + \sum_{k=1}^{n} (a_k \cos kx + b_k \sin kx) ,$$

with the Fourier Coefficients defined by

$$(2.17) \qquad a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos kx dx , \quad b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin kx dx ,$$

is a least square approximation to $f(x)$ with unit weight function, in the interval $[-\pi,\pi]$.

At any interior point x of the interval in which $f(x)$ is bounded and has a finite number of Maxima and Minima and a finite number of non-coincident discontinuities, the Fourier Series converges to $\frac{1}{2}[f(x_+)+f(x_-)]$ which reduces to $f(x)$ at a point of continuity. However, the rate of convergence of the Fourier Series, which in other words is the rate of decrease of its coefficients, depends on the degree of smoothness of the function, measured by the order of the derivative which first becomes discontinuous at any point in the closed interval $[-\pi,\pi]$. Even if $f(x)$ is perfectly smooth, it may have terminal discontinuities with regard to the Fourier theory which in turn affects the rate of convergence of Fourier Series.

Consider the Fourier expansion of the function $f(x)$

defined in the interval $[-1,1]$ and expressed as the sum of even and odd functions $f_1(x) = \frac{1}{2}[f(x)+f(-x)]$ and $f_2(x) = \frac{1}{2}[f(x)-f(-x)]$ respectively. Thus

$$(2.18)\quad \begin{cases} f_1(x) = \frac{1}{2}a_o + \sum\limits_{k=1}^{\infty} a_k \cos kx, & a_k = \frac{2}{\pi}\int_o^{\pi} f_1(x)\cos kx dx\ , \\ f_2(x) = \sum\limits_{k=1}^{\infty} b_k \sin kx, & b_k = \frac{2}{\pi}\int_o^{\pi} f_2(x)\sin kx dx\ . \end{cases}$$

All terms of the sine series vanish at the middle point $x = 0$ where $f_2(x) = 0$ and at the terminal point $x = \pi$ where $f_2(x) = \frac{1}{2}[f(\pi)-f(-\pi)]$. Hence unless $f(\pi) = f(-\pi)$, the series will not converge at the end points of the range and will converge very slowly at the intermediate points. Of course, the first derivative of the cosine series vanishes at the terminal points. But this is far less serious than the discontinuity in the function itself and we should expect the cosine series to converge much faster than the sine series. To be more specific, on integrating by parts, we have

$$(2.19a)\quad \int_o^{\pi} f(x)\cos kx dx = \frac{1}{k^2}[f'(x)\cos kx]_o^{\pi} - \frac{1}{k^2}\int_o^{\pi} f''(x)\cos kx dx\ ,$$

$$(2.19b)\quad \int_o^{\pi} f(x)\sin kx dx = -\frac{1}{k}[f(x)\cos kx]_o^{\pi} + \frac{1}{k}\int_o^{\pi} f'(x)\cos kx dx\ .$$

For large values of k the integrals are likely to be small, being dominated by the oscillations in $\cos kx$. Thus ultimately the cosine series converges like k^{-2} and sine series like k^{-1}.

Considering the range $[-1,1]$ and making the transformation $x = \cos\theta$, so that

(2.20) $$f(x) = f(\cos\theta) = g(\theta), \quad 0 \le \theta \le \pi \ .$$

The function $g(\theta)$ is even and "genuinely" periodic with a period 2π. In addition, if $f(x)$ has a large number of finite derivatives in $[-1,1]$, so has $g(\theta)$ in $[0,\pi]$. Interpretting the Fourier cosine series

(2.21) $$g(\theta) = \frac{1}{2} a_o + \sum_{k=1}^{\infty} a_k \cos k\theta \ , \quad a_k = \frac{2}{\pi}\int_o^{\pi} g(\theta) \cos k\theta d\theta \ ,$$

in terms of x, we produce the Chebyshev Series

(2.22) $$f(x) = \frac{1}{2} a_o + \sum_{k=1}^{\infty} a_k T_k(x) \ , \quad a_k = \frac{2}{\pi}\int_{-1}^{1} (1-x^2)^{-\frac{1}{2}} f(x) T_k(x) dx \ .$$

This has the same convergence properties as the Fourier Series with the additional advantage that the terminal discontinuities are eliminated. Also for sufficiently smooth functions, a_k has the order of magnitude $1/2^{k-1}.(k!)$ to which k^{-2} stands no comparison for sufficiently large values of k.

2.5. Semi-Discrete Solution for $C_o(x,\theta)$ and $T_o(x,\theta)$

Before proceeding with the solution of the system, we wish to prove the

Lemma 2.1. *If*

$$\int e^{-kx}\left(\tfrac{1}{2}\, a_o T_o^* + a_1 T_1^* + \ldots + a_n T_n^*\right) dx$$

(2.23)

$$= e^{-kx}\left(\tfrac{1}{2}\, b_o T_o^* + b_1 T_1^* + \ldots + b_n T_n^*\right) ,$$

we have

(2.24)

$$\boxed{\begin{gathered} b_r = \frac{4(r+1)}{k}\, b_{r+1} + b_{r+2} - \frac{a_r - a_{r+2}}{k} , \\ r = n, n-1, \ldots, 0 \; ; \quad b_{n+1} = b_{n+2} = 0 \; ; \quad a_{n+1} = a_{n+2} = 0 \; . \end{gathered}}$$

Proof: Differentiating both sides of (2.23) with respect to x, we get

$$e^{-kx}\left(\tfrac{1}{2}\, a_o T_o^* + a_1 T_1^* + \ldots + a_n T_n^*\right)$$

$$= -ke^{-kx}\left(\tfrac{1}{2}\, b_o T_o^* + b_1 T_1^* + \ldots + b_n T_n^*\right)$$

$$+ e^{-kx}\left(\tfrac{1}{2}\, b_o' T_o^* + b_1' T_1^* + \ldots + b_{n-1}' T_{n-1}^*\right) ,$$

where

$$b'_{r-1} - b'_{r+1} = 4rb_r \ , \quad r = 1(1)n \quad \text{and} \quad b'_n = b'_{n+1} = 0 \ .$$

Comparing the coefficients,

$$a_r = -kb_r + b'_r \ , \quad r = 0(1)n \ .$$

Therefore,

$$a_{r-1} - a_{r+1} = -k(b_{r-1} - b_{r+1}) + 4rb_r \ ,$$

i.e.

$$b_r = \frac{4(r+1)}{k} b_{r+1} + b_{r+2} - \frac{a_r - a_{r+2}}{k} \ ,$$

$$r = n, n-1, \ldots, 0 \ ; \quad b_{n+1} = b_{n+2} = 0 \ ; \quad a_{n+1} = a_{n+2} = 0 \ .$$

This proves the Lemma.

Reverting to the solution of (1.30), the substitution $x = Ry$ where R is the depth at which concentration and temperature are required, the same are modified to

(2.25) $$\frac{1}{R^2} \frac{d^2 C_o^{(r+1)}}{dy^2} - \alpha C_o^{(r+1)} = -\beta C_o^{(r)} \ ,$$

$$(2.26)\qquad \frac{1}{R^2}\frac{d^2T_o^{(r+1)}}{dy^2} - \gamma T_o^{(r+1)} = -\gamma T_o^{(r)} - \lambda C_o^{(r+1)} ,$$

where $C_o^{(r)} = C_o(y,\theta_r)$, $T_o^{(r)} = T_o(y,\theta_r)$.

The boundary conditions (1.32) are modified to

$$(2.27a)\qquad C_o^{(r)}(0) = f_r , \quad T_o^{(r)}(0) = g_r ,$$

$$(2.27b)\qquad C_o^{(o)}(y) = 0 , \quad T_o^{(o)}(y) = 0 ,$$

$$(2.27c)\qquad \underset{R\to\infty}{\mathrm{Lt}}\ C_o^{(r)}(1) = 0 . \quad \underset{R\to\infty}{\mathrm{Lt}}\ T_o^{(r)}(1) = 0 .$$

For $r = 0$ and 1, the equation (2.25) yields

$$(2.28a)\qquad C_o^{(1)}(y) = f_1\cdot\exp(-R\sqrt{\alpha}\ y) ,$$

$$(2.28b)\qquad C_o^{(2)}(y) = [\frac{\beta f_1}{2\sqrt{\alpha}} Ry+f_2]\ \exp(-R\sqrt{\alpha}\ y) .$$

For general values of r, the solution is of the form

$$(2.29)\qquad C_o^{(r)}(y) = \exp(-R\sqrt{\alpha}\ y) \sum_{n=o}^{r-1}{}' a_{r,n}T_n^*(y) ,$$

where prime in the sigma implies that first term is to be taken by a factor of half.

Multiplying both sides of (2.25) by $\exp(-R\sqrt{\alpha}\ y)$, the

differential equation is made exact and we have

$$\text{(2.30)} \qquad \frac{1}{R^2}\left[\frac{dC_o^{(r+1)}}{dy} + R\sqrt{\alpha}\, C_o^{(r+1)}\right] \exp(-R\sqrt{\alpha}\, y) = -\beta \int e^{-\sqrt{\alpha}\, Ry} C_o^{(r)} dy$$

$$= \exp(-2R\sqrt{\alpha} y) \sum_{n=o}^{r-1}{}' A_{r,n} T_n^*(y) \ ,$$

where the use of Lemma 2.1 and equation (2.29) gives

$$\text{(2.31)} \qquad A_{r,n} = \frac{2(n+1)}{\sqrt{\alpha}\ \ R} A_{r,n+1} + A_{r,n+2} + \beta \frac{a_{r,n} - a_{r,n+2}}{2\sqrt{\alpha}\, R} \ ,$$

$$n = r-1, r-2, \ldots, 0 \ ; \quad A_{r,s} = 0 \ \text{ for } \ s \geq r \ .$$

The constant of integration vanishes by taking the limits as $R \to \infty$.

Equation (2.30) may further be integrated to give

$$\text{(2.32)} \qquad \exp(R\sqrt{\alpha}\ y) C_o^{(r+1)} = R^2 \int \sum_{n=o}^{r-1}{}' A_{r,n} T_n^* dy \ ,$$

$$= \sum_{n=o}^{r}{}' a_{r+1,n} T_n^* \ ,$$

which by use of (A.18) gives

$$\text{(2.33)} \qquad a_{r+1,n} = \frac{R^2 (A_{r,n-1} - A_{r,n+1})}{4n} \ , \quad (n = 1(1)r) \ .$$

Set $y = 0$ in (2.32). Also recall that $C_o^{(r+1)}(0) = f_{r+1}$ whence

$$a_{r+1,o} = 2[f_{r+1} + \sum_{n=1}^{r} a_{r+1,n}(-1)^{n-1}] \ .$$

Combining (2.31) and (2.33) gives

$$a_{r+1,n} = \frac{R}{\sqrt{\alpha}}\left[\frac{1}{2} A_{r,n} + \frac{\beta(a_{r,n-1} - a_{r,n+1})}{8n\sqrt{\alpha}}\right] \ .$$

Changing n to $n+2$, subtracting and utilising (2.33), we get

(2.34)

$$\boxed{\begin{aligned} a_{r+1,n} &= \frac{2(n+1)}{R\sqrt{\alpha}} a_{r+1,n+1} + a_{r+1,n+2} + \frac{R\beta}{8\sqrt{\alpha}}\left[\frac{a_{r,n-1} - a_{r,n+1}}{n} - \frac{a_{r,n+1} - a_{r,n+3}}{n+2}\right] , \\ & n = r(-1)1 \ ; \quad a_{r,s} = 0 \quad \text{for} \quad s \geq r \ ; \\ a_{r+1,o} &= 2[f_{r+1} + \sum_{n=1}^{r} a_{r+1,n}(-1)^{n-1}] . \end{aligned}}$$

This determines $C_o^{(r+1)}$ from $C_o^{(r)}$.

If the whole time interval is divided into p equal parts,

we have finally

$$C_o(y=1) = [\exp(-R\sqrt{\alpha}\ y) \sum_{n=o}^{p-1}{}' a_{p,n} T_n^*(y)]_{y=1} \tag{2.35}$$

$$= \exp(-R\sqrt{\alpha}) \sum_{n=o}^{p-1}{}' a_{p,n} \ .$$

Now to determine $T_o(y,\theta_r)$ for $r = 0$, the equation (2.26) yields

$$T_o^{(1)}(y) = (g_1 + \frac{\lambda f_1}{\alpha-\gamma}) \exp(-R\sqrt{\gamma}\ y) - \frac{\lambda f_1}{\alpha-\gamma} \exp(-R\sqrt{\alpha}\ y) \ . \tag{2.36}$$

For general values of r, the solution of (2.26) is of the form

$$T_o^{(r)}(y) = \exp(-R\sqrt{\gamma}\ y) \sum_{n=o}^{r-1}{}' b_{r,n} T_n^* + \exp(-R\sqrt{\alpha}\ y) \sum_{n=o}^{r-1}{}' c_{r,n} T_n^* \ . \tag{2.37}$$

Equation (2.26) may now be expressed as

$$\frac{1}{R^2} \frac{d}{dy} [\exp(-R\sqrt{\gamma}\ y)\{\frac{dT_o^{(r+1)}}{dy} + \sqrt{\gamma}\ RT_o^{(r+1)}\}] \tag{2.38}$$

$$= -\gamma \exp(-2R\sqrt{\gamma}\ y) \sum_{n=o}^{r-1}{}' b_{r,n} T_n^* - \gamma \exp(-R\nu y) \sum_{n=o}^{r-1}{}' c_{r,n} T_n^*$$

$$- \lambda \exp(-R\nu y) \sum_{n=o}^{r}{}' a_{r+1,n} T_n^*$$

$$= -\gamma \exp(-2R\sqrt{\gamma}\,y) \sum_{n=o}^{r-1}{}' b_{r,n}T_n^* + \exp(-R\nu y) \sum_{n=o}^{r}{}' d_{r+1,n}T_n^* ,$$

where

(2.39) $$d_{r+1,n} = -\gamma c_{r,n} - \lambda a_{r+1,n} , \quad n = 0(1)r .$$

Integrating (2.38),

(2.40) $$\frac{1}{R^2} \exp(-R\sqrt{\gamma}\,y)\left(\frac{dT_o^{(r+1)}}{dy} + R\sqrt{\gamma}\,T_o^{(r+1)}\right)$$

$$= \exp(-2R\sqrt{\gamma}\,y) \sum_{n=o}^{r-1}{}' B_{r,n}T_n^* + \exp(-R\nu y) \sum_{n=o}^{r}{}' D_{r+1,n}T_n^* ,$$

where taking limits, as $R \to \infty$, the constant of integration again vanishes. Also the use of Lemma 2.1 yields

(2.41a) $$B_{r,n} = \frac{2(n+1)}{\sqrt{\gamma}\,R} B_{r,n+1} + B_{r,n+2} + \sqrt{\gamma}\,\frac{b_{r,n}-b_{r,n+2}}{2R} ,$$

(2.41b) $$D_{r+1,n} = \frac{4(n+1)}{\nu R} D_{r+1,n+1} + D_{r+1,n+2} - \frac{d_{r+1,n}-d_{r+1,n+2}}{\nu R} .$$

Multiplying both sides of (2.40) by $R^2 \exp(2R\sqrt{\gamma}\,y)$ and integrating, we have

$$\exp(R\sqrt{\gamma}\,y)T_o^{(r+1)} = \sum_{n=o}^{r}{}' b_{r+1,n}T_n^* + \exp[(\sqrt{\gamma} - \sqrt{\alpha})Ry] \sum_{n=o}^{r}{}' c_{r+1,n}T_n^* ,$$

that is,

$$(2.42) \qquad T_o^{(r+1)} = \exp(-R\sqrt{\gamma}\, y) \sum_{n=o}^{r}{}' \, b_{r+1,n} T_n^* + \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r}{}' \, c_{r+1,n} T_n^* \, ,$$

where

$$(2.43a) \qquad b_{r+1,n} = \frac{R^2(B_{r,n-1} - B_{r,n+1})}{4n} \, , \quad n = 1(1)r \, ,$$

$$(2.43b) \qquad c_{r+1,n} = \frac{4(n+1)}{(\sqrt{\alpha} - \sqrt{\gamma})R} c_{r+1,n+1} + c_{r+1,n+2} - \frac{R(D_{r+1,n} - D_{r+1,n+2})}{\sqrt{\alpha} - \sqrt{\gamma}} \, , \quad n = 0(1)r \, .$$

In (2.42) set $y = 0$. Also recall that $T_o^{(r+1)}(y=0) = g_{r+1}$ whence

$$(2.44) \qquad \boxed{b_{r+1,o} = 2[g_{r+1} + \sum_{n=1}^{r} b_{r+1,n}(-1)^{n-1} + \sum_{n=o}^{r}{}' \, c_{r+1,n}(-1)^{n-1}] \, .}$$

Combining (2.41a) and (2.43a),

$$b_{r+1,n} = \frac{R}{2\sqrt{\gamma}} B_{r,n} + R\sqrt{\gamma}\, \frac{b_{r,n-1} - b_{r,n+1}}{8n} \, .$$

Changing n to n + 2, subtracting and using (2.41a), we get

$$\boxed{\begin{aligned} b_{r+1,n} &= \frac{2(n+1)}{R\sqrt{\gamma}} b_{r+1,n+1} + b_{r+1,n+2} \\ &\quad + \frac{R\sqrt{\gamma}}{8}\left[\frac{b_{r,n-1}-b_{r,n+1}}{n} - \frac{b_{r,n+1}-b_{r,n+3}}{n+2}\right], \\ & n = r(-1)1\ ;\ b_{rs} = 0 \text{ for } s \geq r\ . \end{aligned}} \tag{2.45}$$

Now using (2.41b) in (2.43b), we get

$$c_{r+1,n} = \frac{4(n+1)}{(\sqrt{\alpha}-\sqrt{\gamma})R} c_{r+1,n+1} + c_{r+1,n+2}$$

$$- \frac{1}{(\sqrt{\alpha}-\sqrt{\gamma})\nu}[4(n+1)D_{r+1,n+1}-(d_{r+1,n}-d_{r+1,n+2})] ,$$

that is,

$$D_{r+1,n+1} = -\frac{(\alpha-\gamma)(c_{r+1,n}-c_{r+1,n+2})}{4(n+1)} + \frac{\nu}{R} c_{r+1,n+1}$$

$$+ \frac{d_{r+1,n}-d_{r+1,n+2}}{4(n+1)} .$$

Using this result in (2.41b) and substituting for $d_{r,n}$ from (2.39), we get

$$
\boxed{\begin{aligned}
c_{r+1,n} &= \left[\frac{4(n+1)}{(\sqrt{\alpha}-\sqrt{\gamma})R}+\frac{4(n+1)}{\nu R}\right](c_{r+1,n+1}-c_{r+1,n+3}) \\
&+\left[1+\frac{16(n+1)(n+2)}{R^2(\alpha-\gamma)}\right]c_{r+1,n+2}+\frac{n+1}{n+3}(c_{r+1,n+2}-c_{r+1,n+4}) \\
&-\frac{\gamma}{\alpha-\gamma}\left[(c_{r,n}-c_{r,n+2})-\frac{n+1}{n+3}(c_{r,n+2}-c_{r,n+4})\right] \\
&-\frac{\lambda}{\alpha-\gamma}\left[(a_{r+1,n}-a_{r+1,n+2})-\frac{n+1}{n+3}(a_{r+1,n+2}-a_{r+1,n+4})\right], \\
&n=r(-1)0\ ;\quad c_{rs}=0 \quad \text{for} \quad s\geq r\ .
\end{aligned}} \tag{2.46}
$$

Relations (2.44), (2.45) and (2.46) determine completely $T_o^{(r+1)}(y)$ from $T_o^{(r)}(y)$.

The whole time interval was divided into p equal parts. Hence finally we get

$$
\begin{aligned}
T_o(y{=}1) &= \left[\exp(-R\sqrt{\gamma}\,y)\sum_{n=o}^{p-1}{}' b_{p,n}T_n^* + \exp(-R\sqrt{\alpha}\,y)\sum_{n=o}^{p-1}{}' c_{p,n}T_n^*\right]_{y=1} \\
&= \exp(-R\sqrt{\gamma})\sum_{n=o}^{p-1}{}' b_{p,n} + \exp(-R\sqrt{\alpha})\sum_{n=o}^{p-1}{}' c_{p,n}\ .
\end{aligned} \tag{2.47}
$$

2.6. Semi-Discrete Solution for $C_1(x,\theta)$

Again the substitution $x = Ry$ in (1.45) leads to

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$$(2.48)\quad \frac{1}{R^2}\frac{d^2C_1^{(r+1)}}{dy^2} - \alpha C_1^{(r+1)} = -\beta C_1^{(r)} + T_o^{(r+1)}C_o^{(r+1)}$$

$$= -\beta C_1^{(r)} + \exp(-R\nu y)\sum_{n=o}^{2r}{}' \ell_{r+1,n}T_n^*$$

$$+ \exp(-2R\sqrt{\alpha}\ y)\sum_{n=o}^{2r}{}' m_{r+1,n}T_n^* ,$$

where

$$(2.49a)\quad \sum_{n=o}^{2r}{}' b_{r+1,n}T_n^* = (\sum_{n=o}^{r}{}' a_{r+1,n}T_n^*)(\sum_{n=o}^{r}{}' \ell_{r+1,n}T_n^*) ,$$

$$(2.49b)\quad \sum_{n=o}^{2r}{}' m_{r+1,n}T_n^* = (\sum_{n=o}^{r}{}' a_{r+1,n}T_n^*)(\sum_{n=o}^{r}{}' c_{r+1,n}T_n^*) .$$

Since the functions $C_o^{(r)}(y)$ were chosen to satisfy the boundary conditions (1.32), the corresponding boundary conditions on $C_1^{(r)}(y)$ are zero conditions.

For $r = 0$, the solution $C_1^{(1)}(y)$ of equation (2.48) is

$$(2.50a)\quad C_1^{(1)}(y) = A\exp(-R\sqrt{\alpha}\ y) + \frac{f_1}{\nu^2-\alpha}(g_1 + \frac{\lambda f_1}{\alpha-\gamma})\exp(-R\nu y)$$

$$- \frac{\lambda f_1^2}{3\alpha(\alpha-\gamma)}\exp(-2R\sqrt{\alpha}\ y) ,$$

where

$$A = -\frac{f_1}{\nu^2-\alpha}\,(g_1+\frac{\lambda f_1}{\alpha-\gamma}) + \frac{\lambda f_1^2}{3\alpha(\alpha-\gamma)} .$$

For general values of r, the solution of (2.48) may be expressed in the form

$$(2.51) \qquad C_1^{(r)}(y) = \exp(-R\sqrt{\alpha}\,y) \sum_{n=o}^{r-1}{}' u_{r,n}T_n^* + \exp(-R\nu y) \sum_{n=o}^{2r-2}{}' v_{r,n}T_n^*$$

$$+ \exp(-2R\sqrt{\alpha}\,y) \sum_{n=o}^{2r-2}{}' w_{r,n}T_n^* .$$

Thus (2.48) takes the form

$$(2.52) \qquad \frac{1}{R^2}\frac{d^2C_1^{(r+1)}}{dy^2} - \alpha C_1^{(r+1)} = -\beta \exp(-R\sqrt{\alpha}\,y) \sum_{n=o}^{r-1}{}' u_{r,n}T_n^*$$

$$+ \exp(-R\nu y) \sum_{n=o}^{2r}{}' p_{r+1,n}T_n^* + \exp(-2R\sqrt{\alpha}\,y) \sum_{n=o}^{2r}{}' q_{r+1,n}T_n^* ,$$

where

$$(2.53a) \qquad p_{r+1,n} = -\beta v_{r,n} + \ell_{r+1,n} ,$$

$$(2.53b) \qquad q_{r+1,n} = -\beta w_{r,n} + m_{r+1,n} , \quad n = 0(1)2r .$$

To make it exact, multiplying both sides of (2.52), by $\exp(-R\sqrt{\alpha}\,y)$ and integrating, we get

$$(2.54)\quad \frac{1}{R^2}\exp(-R\sqrt{\alpha}\,y)\left(\frac{dC_1^{(r+1)}}{dy} + R\sqrt{\alpha}\,C_1^{(r+1)}\right)$$

$$= \exp(-2R\sqrt{\alpha}\,y)\sum_{n=o}^{r-1}{}' U_{r,n}T_n^* + \exp[-(\nu+\sqrt{\alpha})Ry]\sum_{n=o}^{2r}{}' P_{r+1,n}T_n^*$$

$$+ \exp(-3R\sqrt{\alpha}\,y)\sum_{n=o}^{2r}{}' Q_{r+1,n}T_n^* \;,$$

where

$$(2.55a)\quad U_{r,n} = \frac{2(n+1)}{\sqrt{\alpha}\,R}U_{r,n+1} + U_{r,n+2} + \beta\,\frac{u_{r,n}-u_{r,n+2}}{2\sqrt{\alpha}\;R}\;,$$

$$n = r(-1)0\;,$$

$$(2.55b)\quad P_{r+1,n} = \frac{4(n+1)}{(\nu+\sqrt{\alpha})R}P_{r+1,n+1} + P_{r+1,n+2} - \frac{p_{r+1,n}-p_{r+1,n+2}}{(\nu+\sqrt{\alpha})R}\;,$$

$$n = 2r(-1)0\;,$$

$$(2.55c)\quad Q_{r+1,n} = \frac{4(n+1)}{3\sqrt{\alpha}\;R}Q_{r+1,n+1} + Q_{r+1,n+2} - \frac{q_{r+1,n}-q_{r+1,n+2}}{3\sqrt{\alpha}\;R}\;,$$

$$n = 2r(-1)0\;,$$

$$(2.55d)\quad U_{r,n} = 0 \;\text{ for }\; n \geq r\;;\; P_{r+1,n} = 0 = Q_{r+1,n} \;\text{ for }\; n \geq 2r\;.$$

The constant of integration vanishes because each term in the limit approaches zero as R approaches infinity.

Again multiplying each side of (2.54) by $\exp(2R\sqrt{\alpha}\, y)$ and integrating, we get

$$(2.56)\qquad C_1^{(r+1)} \exp(R\sqrt{\alpha}\, y) = \sum_{n=o}^{r}{}' u_{r+1,n}T_n^* + \exp(-R\sqrt{\gamma}\, y) \sum_{n=o}^{2r}{}' v_{r+1,n}T_n^*$$

$$+ \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{2r}{}' w_{r+1,n}T_n^* ,$$

which after using (2.55) simplifies to

$$(2.57a)\qquad u_{r+1,n} = \frac{R}{2\sqrt{\alpha}} U_{r,n} + R\beta \frac{u_{r,n-1}-u_{r,n+1}}{8n\sqrt{\alpha}} , \quad n = r(-1)1 ,$$

$$(2.57b)\qquad v_{r+1,n} = \frac{4(n+1)}{\sqrt{\gamma}\, R} v_{r+1,n+1} + v_{r+1,n+2}$$

$$- \frac{1}{\sqrt{\gamma}\,(\nu+\sqrt{\alpha})} [4(n+1)P_{r+1,n+1}-(p_{r+1,n}-p_{r+1,n+2})] ,$$

$$n = 2r(-1)0 ,$$

$$(2.57c)\qquad w_{r+1,n} = \frac{4(n+1)}{\sqrt{\alpha}\, R} w_{r+1,n+1} + w_{r+1,n+2}$$

$$- \frac{1}{3\alpha} [4(n+1)Q_{r+1,n+1}-(q_{r+1,n}-q_{r+1,n+2})] ,$$

$$n = 2r(-1)0 .$$

Using (2.49), (2.53), (2.55) and (2.57), we get the

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sets of coefficients $\{u_{r+1,n} \mid n = 1(1)r\}$, $\{v_{r+1,n} \mid n = 1(1)2r\}$ and $\{w_{r+1,n} \mid n = 1(1)2r\}$. However, direct results may be obtained by eliminating U_{rn}, P_{rn}, Q_{rn} from (2.55) and (2.57). In addition to that, substitution for p_{rn}, q_{rn} from (2.53) yields the recurrsion formulae

$$(2.58a)\quad u_{r+1,n} = \frac{2(n+1)}{R\sqrt{\alpha}} u_{r+1,n+1} + u_{r+1,n+2} + \frac{\beta R}{8\sqrt{\alpha}} \left[\frac{u_{r,n-1}-u_{r,n+1}}{n} - \frac{u_{r,n+1}-u_{r,n+3}}{n+2}\right] ,$$

$$n = 1(1)r ,$$

$$(2.58b)\quad v_{r+1,n} = \left[1- \frac{16(n+1)(n+2)}{R^2\sqrt{\gamma}\,(\nu+\sqrt{\alpha})}\right]v_{r+1,n+2} + \frac{8(n+1)}{R\sqrt{\gamma}\,(\nu+\sqrt{\alpha})} (v_{r+1,n+1} - v_{r+1,n+3}) + \frac{n+1}{n+3} (v_{r+1,n+2}-v_{r+1,n+4}) - \frac{\beta}{\sqrt{\gamma}\,(\nu+\sqrt{\alpha})} \left[(v_{r,n} - v_{r,n+2}) - \frac{n+1}{n+3} (v_{r,n+2}-v_{r,n+4})\right]$$

$$+ \frac{1}{\sqrt{\gamma}(\nu+\sqrt{\alpha})} \left[(\ell_{r+1,n}-\ell_{r+1,n+2}) - \frac{n+1}{n+3} (\ell_{r+1,n+2}-\ell_{r+1,n+4})\right] ,$$

$$n = 0(1)2r ,$$

$$(2.58c)\quad w_{r+1,n} = \left[1- \frac{16(n+1)(n+2)}{3R^2\alpha}\right]w_{r+1,n+2} + \frac{16(n+1)}{3R\sqrt{\alpha}} (w_{r+1,n+1}-w_{r+1,n+3}) + \frac{n+1}{n+3} (w_{r+1,n+2}-w_{r+1,n+4}) - \frac{\beta}{3\alpha} [(w_{r,n}-w_{r,n+2})$$

$$- \frac{n+1}{n+3} (w_{r,n+2} - w_{r,n+4})] + \frac{1}{3\alpha} [(m_{r+1,n} - m_{r+1,n+2})$$

$$- \frac{n+1}{n+3} (m_{r+1,n+2} - m_{r+1,n+4})] ,$$

$$n = 0(1)2r .$$

In (2.51) change r to $r + 1$, set $y = 0$ and recall that $C_1^{(r+1)}(0) = 0$. This gives

$$\text{(2.58d)} \qquad u_{r+1,o} = 2[\sum_{n=1}^{r} u_{r+1,n}(-1)^{n-1} + \sum_{n=o}^{2r}{}' v_{r+1,n}(-1)^{n-1}$$

$$+ \sum_{n=o}^{2r}{}' w_{r+1,n}(-1)^{n-1}].$$

This determines $C_1^{(r+1)}$ from $C_1^{(r)}$, $C_o^{(r+1)}$ and $T_o^{(r+1)}$.

At the expiry of the time interval, that is, after p time increments, we have

$$\text{(2.59)} \qquad C_1(y=1) = \exp(-R\sqrt{\alpha}) \sum_{n=o}^{p-1}{}' u_{p,n} + \exp(-R\nu) \sum_{n=o}^{2p-2}{}' v_{p,n}$$

$$+ \exp(-2R\sqrt{\alpha}) \sum_{n=o}^{2p-2}{}' w_{p,n} .$$

CHAPTER III

SIMPLIFICATION OF SOLUTION IN CHEBYSHEV SERIES

3.1. General

In the last chapter, recursion relations have been derived to give the coefficients associated with the next-step differential equation in terms of the same of the previous-step solution. In the present chapter, these relations have been expressed in a much simpler and direct manner by employing matrices. The next-step solution depends upon the derivation of the inverse of next-order matrix from the previous-step matrix. The matrices are lower triangular and therefore it is not difficult to find their inverses by the Gauss Elimination method. However, they are generated in a particular manner which makes it convenient to derive the inverse of $(r+1)$th order matrix from that of rth order matrix. Thus stepping to the next stage amounts to extension of these matrices by the addition of last row, the last column except for the diagonal element in each case being that of zeroes. Although the present technique is much simpler for automatic programming on a digital computer, it will be observed that it is not as fast for a desk calculator for which the relations of the last chapter are more direct and easier to handle.

Any apparent difference between the results of the last chapter and this chapter is only superficial. In the last chapter, the (r+1)th step coefficients were expressed in backward recursion relation in terms of the (r+1)th step coefficients which follow and the rth step coefficients which were known. If the recursion relations are conclusively employed so that (r+1)th step coefficients are expressed in terms of the rth step coefficients only,we have the relations of the present chapter. Thus, in case there is no round-off error, the results of the last and present chapter must agree.

3.2. Semi-Discrete Solution for $C_o(x,\theta)$ and $T_o(x,\theta)$

Reverting to the solution of (2.25), viz.

$$\frac{1}{R^2}\frac{d^2C_o^{(r+1)}}{dy^2} - \alpha C_o^{(r+1)} = -\beta C_o^{(r)} , \tag{3.1}$$

let

$$C_o^{(r)} = \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r-1}{}' a_{r,n} T_n^*(y) , \tag{3.2a}$$

$$C_o^{(r+1)} = \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r}{}' a_{r+1,n} T_n^*(y) . \tag{3.2b}$$

Substituting in the above and comparing coefficients, we get

$$
(3.3)\quad \left\{
\begin{array}{ll}
-\dfrac{2\sqrt{\alpha}}{R}\, a'_{r+1,o} + \dfrac{1}{R^2}\, a''_{r+1,o} & = -\beta a_{r,o}\ , \\[2ex]
-\dfrac{2\sqrt{\alpha}}{R}\, a'_{r+1,1} + \dfrac{1}{R^2}\, a''_{r+1,1} & = -\beta a_{r,1}\ , \\[2ex]
\cdots\cdots\cdots\cdots\cdots & \\
\cdots\cdots\cdots\cdots\cdots & \\[2ex]
-\dfrac{2\sqrt{\alpha}}{R}\, a'_{r+1,r-2} + \dfrac{1}{R^2}\, a''_{r+1,r-2} & = -\beta a_{r,r-2}\ , \\[2ex]
-\dfrac{2\sqrt{\alpha}}{R}\, a'_{r+1,r-1} & = -\beta a_{r,r-1}\ ,
\end{array}
\right.
$$

where primes denote differentials w.r.t. y in the sense of relations (A-23) and (A-24). Above relations can be combined into a single relation

$$
(3.4a)\qquad -\frac{2\sqrt{\alpha}}{R}\, a'_{r+1,n} + \frac{1}{R^2}\, a''_{r+1,n} = -\beta a_{r,n}\ ,
$$

$$
(3.4b)\qquad n = 0(1)r-1\ ;\quad a''_{r+1,r-1} = 0\ .
$$

Using relations (A-23) and (A-24), we get

$$
\begin{aligned}
(3.5)\qquad & -\frac{2\sqrt{\alpha}}{R}\, 4[(n+1)a_{r+1,n+1}+(n+3)a_{r+1,n+3}+(n+5)a_{r+1,n+5}+\ldots] \\
& + \frac{4^2}{R^2}\, [(n+1)(n+2)a_{r+1,n+2}+2(n+2)(n+4)a_{r+1,n+4} \\
& + 3(n+3)(n+6)a_{r+1,n+6}+\ldots] = -\beta a_{r,n}\ ,
\end{aligned}
$$

where the series in each case terminates because $a_{p,q} = 0$ for $q \geq p$.

Put $n = 0,1,2,\ldots,r-1$, to get

$$(3.6a)\qquad -\frac{2\sqrt{\alpha}}{R}\,4[1\cdot a_{r+1,1}+3a_{r+1,3}+5a_{r+1,5}+\ldots]$$

$$+\frac{16}{R^2}[1.1.2a_{r+1,2}+2.2.4a_{r+1,4}+3.3.6a_{r+1,6}+\ldots] = -\beta a_{r,o} ,$$

$$(3.6b)\qquad -\frac{2\sqrt{\alpha}}{R}\,4[2a_{r+1,2}+4a_{r+1,4}+6a_{r+1,6}+\ldots]$$

$$+\frac{16}{R^2}[1.2.3a_{r+1,3}+2.3.5a_{r+1,5}+3.4.7a_{r+1,7}+\ldots] = -\beta a_{r,1} ,$$

$$(3.6c)\qquad -\frac{2\sqrt{\alpha}}{R}\,4[3a_{r+1,3}+5a_{r+1,5}+7a_{r+1,7}+\ldots]$$

$$+\frac{16}{R^2}[1.3.4a_{r+1,4}+2.4.6a_{r+1,6}+3.5.8a_{r+1,8}+\ldots] = -\beta a_{r,2} ,$$

and etc. These equations can be arranged in the matrix form as

$$(3.7)\qquad (a_{r+1,1}a_{r+1,2}a_{r+1,3}\ \cdots\ a_{r+1,r}) \times A_r$$

$$= \frac{\beta R^2}{16}(a_{r,o}a_{r,1}a_{r,2}\ \cdots\ a_{r,r-1}) ,$$

where A is a matrix of order r, viz.

$$(3.8) \qquad A_r = \begin{bmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ -1.1.2 & 2\varepsilon_1 & 0 & 0 & 0 & 0 & \cdots \\ 3\varepsilon_1 & -1.2.3 & 3\varepsilon_1 & 0 & 0 & 0 & \cdots \\ -2.2.4 & 4\varepsilon_1 & -1.3.4 & 4\varepsilon_1 & 0 & 0 & \cdots \\ 5\varepsilon_1 & -2.3.5 & 5\varepsilon_1 & -1.4.5 & 5\varepsilon_1 & 0 & \cdots \\ -3.3.6 & 6\varepsilon_1 & -2.4.6 & 6\varepsilon_1 & -1.5.6 & 6\varepsilon_1 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}_{r\times r} ,$$

and

$$(3.9) \qquad \varepsilon_1 = R\sqrt{\alpha}/2 .$$

This gives the recursion relation

$$(3.10a) \qquad \boxed{\begin{aligned} &(a_{r+1,1}\ a_{r+1,2}\ a_{r+1,3}\ \cdots\ a_{r+1,r}) \\ &\qquad = \frac{\beta R^2}{16}(a_{r,o}\ a_{r,1}\ \cdots\ a_{r,r-1})\quad A_r^{-1} , \end{aligned}}$$

where A_r^{-1} is again a lower triangular matrix, the inverse of lower triangular matrix A_r .

In (3.2b), set $y = 0$ and recall that $C_o^{(r+1)} = f_{r+1}$. This gives

(3.10b) $$\boxed{a_{r+1,o} = 2(f_{r+1}+a_{r+1,1}-a_{r+1,2}+a_{r+1,3} \ldots) .}$$

Equations (3.10a) and (3.10b) derive $C_o^{(r+1)}$ from $C_o^{(r)}$.

Finally, as in (2.35),

(3.11) $$C_o(y=1) = \exp(-R\sqrt{\alpha}) \sum_{n=o}^{p-1}{}' a_{p,n} .$$

To solve (2.26), viz.

(3.12) $$\frac{1}{R^2}\frac{d^2T_o^{(r+1)}}{dy^2} - \gamma T_o^{(r+1)} = -\gamma T_o^{(r)} - \lambda C_o^{(r+1)} , \quad 0 \leq y \leq 1,$$

let

(3.13a) $$T_o^{(r)} = \exp(-R\sqrt{\gamma}\, y) \sum_{n=o}^{r-1}{}' b_{r,n}T_n^*(y) + \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r-1}{}' c_{r,n}T_n^*(y) ,$$

(3.13b) $$T_o^{(r+1)} = \exp(-R\sqrt{\gamma}\, y) \sum_{n=o}^{r}{}' b_{r+1,n}T_n^*(y) + \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r}{}' c_{r+1,n}T_n^*(y).$$

Substituting in the above and comparing coefficients, we get

(3.14) $$\exp(-R\sqrt{\gamma}\, y)\left[\frac{-2\sqrt{\gamma}}{R} b'_{r+1,n} + \frac{1}{R^2} b''_{r+1,n}\right]$$

$$+ \exp(-R\sqrt{\alpha}\, y)\left[(\alpha-\gamma)c_{r+1,n} - \frac{2\sqrt{\alpha}}{R} c'_{r+1,n} + \frac{1}{R^2} c''_{r+1,n}\right]$$

$$= - \exp(-R\sqrt{\gamma}\, y)\gamma b_{r,n} - \exp(-R\sqrt{\alpha}\, y)(\gamma c_{r,n}+\lambda a_{r+1,n}) .$$

But α and γ are independent of each other. Thus, equating the coefficients of $\exp(-R\sqrt{\alpha}\, y)$ and $\exp(-R\sqrt{\gamma}\, y)$, we get

(3.15a) $$\frac{-2\sqrt{\gamma}}{R} b'_{r+1,n} + \frac{1}{R^2} b''_{r+1,n} = -\gamma b_{r,n} ,$$

(3.15b) $$(\alpha-\gamma)c_{r+1,n} - \frac{2\sqrt{\alpha}}{R} c'_{r+1,n} + \frac{1}{R^2} c''_{r+1,n} = -\gamma c_{r,n} - \lambda\, a_{r+1,n} .$$

Using (A-23) and (A-24), above are expressed in the form

(3.16a) $$\frac{-2\sqrt{\gamma}}{R} 4[(n+1)b_{r+1,n+1}+(n+3)b_{r+1,n+3}+(n+5)b_{r+1,n+5}+ \ldots]$$

$$+ \frac{16}{R^2} [(n+1)(n+2)b_{r+1,n+2}+2(n+2)(n+4)b_{r+1,n+4}$$

$$+ 3(n+3)(n+6)b_{r+1,n+6}+\ldots] = -\gamma b_{r,n} ,$$

(3.16b) $$(\alpha-\gamma)c_{r+1,n} - \frac{2\sqrt{\alpha}}{R} 4[(n+1)c_{r+1,n+1}+(n+3)c_{r+1,n+3}+(n+5)c_{r+1,n+5}+\ldots]$$

$$+ \frac{16}{R^2} [1(n+1)(n+2)c_{r+1,n+2}+2(n+2)(n+4)c_{r+1,n+4}$$

$$+ 3(n+3)(n+6)c_{r+1,n+6}+\ldots] = -\gamma c_{r,n} - \lambda\, a_{r+1,n} .$$

Set $n = 0,1,2,\ldots,r-1$ and $n = 0,1,2,\ldots,r$, to get

$$(3.17a)\qquad (b_{r+1,1}\ b_{r+1,3}\ \ldots,b_{r+1,r})B_r$$

$$= \frac{\gamma R^2}{16}\,(b_{r,o}\ b_{r,1}\ b_{r,2}\ \cdots\ b_{r,r-1})\ ,$$

$$(3.17b)\qquad (c_{r+1,o}\ c_{r+1,1}\ c_{r+1,2}\ \ldots,c_{r+1,r})C_{r+1}$$

$$= \frac{\gamma R^2}{16}\,(c_{r,o}\ c_{r,1}\ c_{r,2},\ldots,c_{r,r-1},0)$$

$$+ \frac{\lambda R^2}{16}\,(a_{r+1,o}\ a_{r+1,1}\ a_{r+1,2}\ \ldots,a_{r+1,r})\ ,$$

where B_r and C_{r+1} are again both lower triangular matrices, viz.

$$(3.18a)\qquad B_r = \begin{bmatrix} \varepsilon_2 & 0 & 0 & 0 & 0 & 0 & \ldots \\ -1.2 & 2\varepsilon_2 & 0 & 0 & 0 & 0 & \ldots \\ 3\varepsilon_2 & -1.2.3 & 3\varepsilon_2 & 0 & 0 & 0 & \ldots \\ -2.2.4 & 4\varepsilon_2 & -1.3.4 & 4\varepsilon_2 & 0 & 0 & \ldots \\ 5\varepsilon_2 & -2.3.5 & 5\varepsilon_2 & -1.4.5 & 5\varepsilon_2 & 0 & \ldots \\ -3.3.6 & 6\varepsilon_2 & -2.4.6 & 6\varepsilon_2 & -1.5.6 & 6\varepsilon_2 & \ldots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \ldots \end{bmatrix}_{r\times r}\ ,$$

$$(3.18b) \quad C_{r+1} = \begin{bmatrix} \xi_1 & 0 & 0 & 0 & 0 & 0 \ldots \\ \varepsilon_1 & \xi_1 & 0 & 0 & 0 & 0 \ldots \\ -1.2 & 2\varepsilon_1 & \xi_1 & 0 & 0 & 0 \ldots \\ 3\varepsilon_1 & -1.2.3 & 3\varepsilon_1 & \xi_1 & 0 & 0 \ldots \\ -2.2.4 & 4\varepsilon_1 & -1.3.4 & 4\varepsilon_1 & \xi_1 & 0 \ldots \\ 5\varepsilon_1 & -2.3.5 & 5\varepsilon_1 & -1.4.5 & 5\varepsilon_1 & \xi_1 \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{bmatrix}_{r+1\times r+1},$$

where

$$(3.19) \qquad \xi_1 = \frac{-(\alpha-\gamma)R^2}{16}, \quad \varepsilon_2 = \frac{R\sqrt{\gamma}}{2}.$$

It may be noted that B_r may be obtained form A_r by replacing ε_1 by ε_2; C_{r+1} is A_r with a diagonal of ξ_1's injected.

Thus we have

$$(3.20a) \qquad \boxed{\begin{aligned} &(b_{r+1,1}\ b_{r+1,2} \cdots b_{r+1,r}) \\ &\quad = \frac{\gamma R^2}{16}(b_{r,o}\ b_{r,1}\ b_{r,2} \cdots b_{r,r-1})B_r^{-1}, \\ &(c_{r+1,o}\ c_{r+1,1} \cdots c_{r+1,r}) = \frac{R^2}{16}[\gamma(c_{r,o}c_{r,1}c_{r,2}\cdots c_{r,r-1},0) \\ &\quad + \lambda(a_{r+1,o}a_{r+1,1}a_{r+1,2} \cdots a_{r+1,r})]C_{r+1}^{-1}. \end{aligned}}$$

(3.20b)

In (3.13b), set $y = 0$ and recall that $T_o^{(r+1)} = g_{r+1}$. This gives

$$\boxed{b_{r+1,o} = 2[(g_{r+1}+b_{r+1,1}-b_{r+1,2}+\ldots) - \frac{1}{2}c_{r+1,o} + (c_{r+1,1}-c_{r+1,2}+c_{r+1,3}-\ldots)].} \tag{3.20c}$$

Equations (3.20a) to (3.20c) derive $T_o^{(r+1)}$ from $T_o^{(r)}$. Finally as in (2.47),

$$T_o(y=1) = \exp(-R\sqrt{\gamma}) \sum_{n=o}^{p-1}{}' b_{p,n} + \exp(-R\sqrt{\alpha}) \sum_{n=o}^{p-1}{}' c_{p,n} . \tag{3.21}$$

3.3. Semi-Discrete Solution for $C_1(x,\theta)$

To solve (2.48) for $C_1(x,\theta_r) = c_1^{(r)}(x)$, viz.

$$\frac{1}{R^2}\frac{d^2C_1^{(r+1)}}{dy^2} - \alpha C_1^{(r+1)} = -\beta C_1^{(r)} + T_o^{(r+1)}C_o^{(r+1)} . \tag{3.22}$$

Let

$$C_o^{(r+1)}T_o^{(r+1)} = \exp(-R\sqrt{\alpha}\,y) \sum_{n=o}^{r}{}' a_{r+1,n}T_n^* \times [\exp(-R\sqrt{\gamma}\,y) \sum_{n=o}^{r}{}' b_{r+1,n}T_n^* \tag{3.23}$$

$$+ \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r}{}' c_{r+1,n} T_n^*]$$

$$= \exp(-R\nu y) \sum_{n=o}^{2r}{}' \ell_{r+1,n} T_n^* + \exp(-2R\sqrt{\alpha}\, y) \sum_{n=o}^{2r}{}' m_{r+1,n} T_n^* ,$$

where ℓ's and m's are defined in (2.49).

(recall $\nu = \sqrt{\alpha} + \sqrt{\gamma}$)

Hence (3.22) reduces to

$$\text{(3.24)} \qquad \frac{1}{R^2} \frac{d^2 C_1^{(r+1)}}{dy^2} - \alpha C_1^{(r+1)} = -\beta C_1^{(r)} + \exp(-R\nu y) \sum_{n=o}^{2r}{}' \ell_{r+1,n} T_n^* + \exp(-2R\sqrt{\alpha}\, y) \sum_{n=o}^{2r}{}' m_{r+1,n} T_n^* .$$

Since functions $C_o^{(r)}(y)$ were chosen to satisfy the boundary conditions (1.32), the corresponding boundary conditions on $C_1^{(r)}(y)$ are zero conditions.

For $r = 0$, the solution $C_1^{(1)}$ of equation (3.22) is as in (2.50). For general values of r, the solution may be expressed in the form (2.51), viz.

$$\text{(3.25)} \qquad C_1^{(r)}(y) = \exp(-R\sqrt{\alpha}\, y) \sum_{n=o}^{r-1}{}' u_{r,n} T_n^* + \exp(-R\nu y) \sum_{n=o}^{2r-2}{}' v_{r,n} T_n^* + \exp(-2R\sqrt{\alpha}\, y) \sum_{n=o}^{2r-2}{}' w_{r,n} T_n^* ,$$

and a similar result may be found $C_1^{(r+1)}(y)$ by replacing r by $(r+1)$ in the above.

Substituting in (3.24), and comparing the coefficients of exponents followed by comparison of coefficients of like T^*'s, we get the relations

(3.26a) $$-\frac{2\sqrt{\alpha}}{R}u'_{r+1,n}+\frac{1}{R^2}u''_{r+1,n}=-\beta u_{r,n}\ , \quad (n=0(1)r-1)\ ,$$

(3.26b) $$(\gamma+2\sqrt{\alpha\gamma})v_{r+1,n}-\frac{2\nu}{R}v'_{r+1,n}+\frac{1}{R^2}v''_{r+1,n}=-\beta v_{r,n}+\ell_{r+1,n}\ ,$$

$$(n=0(1)2r)\ ,$$

(3.26c) $$3\alpha w_{r+1,n}-\frac{4\sqrt{\alpha}}{R}w'_{r+1,n}+\frac{1}{R^2}w''_{r+1,n}=-\beta w_{r,n}+m_{r+1,n}\ ,$$

$$(n=0(1)2r)\ ,$$

where

(3.26d) $$u_{r+1,n}=0 \quad \text{for} \quad n\geq r\ ;\quad v_{r,n}=0=w_{r,n} \quad \text{for} \quad n>2r-2\ .$$

Again using (A-23) and (A-24), we get

(3.27a) $$\frac{-2\sqrt{\alpha}}{R}4[(n+1)u_{r+1,n+1}+(n+3)u_{r+1,n+3}+(n+5)u_{r+1,n+5}+\ldots]$$

$$+ \frac{16}{R^2}\,[1(n+1)(n+2)u_{r+1,n+2}+2(n+2)(n+4)u_{r+1,n+4}$$

$$+ 3(n+3)(n+6)u_{r+1,n+6}+\ldots] = -\beta u_{r,n}\ ,$$

$$(n = 0(1)r - 1)\ ,$$

(3.27b) $$(\gamma+2\sqrt{\alpha}\gamma)v_{r+1,n} - \frac{2\nu}{R}\,4[(n+1)v_{r+1,n+1}+(n+3)v_{r+1,n+3}+\ldots]$$

$$+ \frac{16}{R^2}\,[1(n+1)(n+2)v_{r+1,n+2}+2(n+2)(n+4)v_{r+1,n+4}$$

$$+ 3(n+3)(n+6)v_{r+1,n+6}+\ldots] = -\beta v_{r,n} + \ell_{r+1,n}\ ,$$

$$(n = 0(1)2r)\ ,$$

(3.27c) $$3\alpha w_{r+1,n} - \frac{4\sqrt{\alpha}}{R}\,4[(n+1)w_{r+1,n+1}+(n+3)w_{r+1,n+3}+(n+5)w_{r+1,n+5}+\ldots]$$

$$+ \frac{16}{R^2}\,[1(n+1)(n+2)w_{r+1,n+2}+2(n+2)(n+4)w_{r+1,n+4}$$

$$+ 3(n+3)(n+6)w_{r+1,n+6}+\ldots] = -\beta w_{r,n} + m_{r+1,n}\ ,$$

$$(n = 0(1)2r)\ .$$

Put $n = 0,1,2,\ldots$ to get

$$(3.28a)\qquad (u_{r+1,1}u_{r+1,2}\cdots u_{r+1,r})A_r = \frac{\beta R^2}{16}(u_{r,o}u_{r,1}\cdots u_{r,r-1}),$$

$$(3.28b)\qquad (v_{r+1,o}v_{r+1,1}\cdots v_{r+1,2r})E_{2r+1} = \frac{\beta R^2}{16}(v_{r,o}v_{r,1}\cdots v_{r,2r-2},0,0) - \frac{R^2}{16}(\ell_{r+1,o}\ell_{r+1,1}\cdots \ell_{r+1,2r}),$$

$$(3.28c)\qquad (w_{r+1,o}w_{r+1,1}\cdots w_{r+1,2r})F_{2r+1} = \frac{\beta R^2}{16}(w_{r,o}w_{r,1}\cdots w_{r,2r-2},0,0) - \frac{R^2}{16}(m_{r+1,o}m_{r+1,1}\cdots m_{r+1,2r}),$$

where

$$(3.29)\qquad E_{2r+1} = \begin{bmatrix} \xi_2 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \varepsilon_{12} & \xi_2 & 0 & 0 & 0 & 0 & \cdots \\ -1.1.2 & 2\varepsilon_{12} & \xi_2 & 0 & 0 & 0 & \cdots \\ 3\varepsilon_{12} & -1.2.3 & 3\varepsilon_{12} & \xi_2 & 0 & 0 & \cdots \\ -2.2.4 & 4\varepsilon_{12} & -1.3.4 & 4\varepsilon_{12} & \xi_2 & 0 & \cdots \\ 5\varepsilon_{12} & -2.3.5 & 5\varepsilon_{12} & -1.4.5 & 5\varepsilon_{12} & \xi_2 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}_{2r+1\times 2r+1},$$

with

$$(3.30)\qquad \xi_2 = \frac{-(\gamma+2\sqrt{\alpha\gamma})R^2}{16},\quad \varepsilon_{12} = \varepsilon_1 + \varepsilon_2,$$

$$(3.31)\quad F_{2r+1} = \begin{bmatrix} \xi_3 & 0 & 0 & 0 & 0 & \cdots \\ 2\varepsilon_1 & \xi_3 & 0 & 0 & 0 & \cdots \\ -1.1.2 & 4\varepsilon_1 & \xi_3 & 0 & 0 & \cdots \\ 6\varepsilon_1 & -1.2.3 & 6\varepsilon_1 & \xi_3 & 0 & \cdots \\ -2.2.4 & 8\varepsilon_1 & -1.3.4 & 8\varepsilon_1 & \xi_3 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}_{2r+1\times 2r+1},$$

with

$$(3.32)\qquad \xi_3 = \frac{-3\alpha R^2}{16}\ .$$

The technique for deriving the matrices E_{2r+1} and F_{2r+1} is similar to that for deriving C_{r+1}. F_{2r+1} may be obtained directly from E_{2r+1} by replacing ξ_2 by ξ_3 and ε_2 by ε_1 .

Thus we have

$$(3.33a)\quad (u_{r+1,1}u_{r+1,2}\ \cdots\ u_{r+1,r}) = \frac{\beta R^2}{16}\,(u_{r,o}u_{r,1}\ \cdots\ u_{r,r-1})A_r^{-1}\ ,$$

$$(3.33b)\quad (v_{r+1,o}v_{r+1,1}\ \cdots\ v_{r+1,2r}) = \frac{R^2}{16}\,[\beta(v_{r,o}v_{r,1}\cdots v_{r,2r-2},0,0)$$

$$- (\ell_{r+1,o}\ell_{r+1,1}\cdots\ \ell_{r+1,2r})]E_{2r+1}^{-1}\ ,$$

$$(3.33c)\quad (w_{r+1,o}w_{r+1,1}\ \cdots w_{r+1,2r}) = \frac{R^2}{16}\,[\beta(w_{r,o}w_{r,1}\cdots w_{r,2r-2},0,0)$$

$$-(m_{r+1,o}m_{r+1,1} \cdots m_{r+1,2r})]F_{2r+1}^{-1} .$$

Recall that $C_1^{(r+1)}(0) = 0$. Hence from (3.25) with r replaced by $r + 1$, we have

$$\text{(3.33d)} \quad u_{r+1,o} = 2[(u_{r+1,1}-u_{r+1,2}+\ldots\pm u_{r+1,r}) - \frac{1}{2}(v_{r+1,o}+w_{r+1,o})$$

$$+ (v_{r+1,1}-v_{r+1,2}+\ldots) + (w_{r+1,1}-w_{r+1,2}+\ldots)] .$$

The equations (3.33) determine $C_1^{(r+1)}(y)$ completely. Finally, as in (2.59),

$$\text{(3.34)} \qquad C_1(y=1) = \exp(-R\sqrt{\alpha}) \sum_{n=o}^{p-1}{}' u_{p,n} + \exp(-R\nu) \sum_{n=o}^{2p-2}{}' v_{p,n}$$

$$+ \exp(-2R\sqrt{\alpha}) \sum_{n=o}^{2p-2}{}' w_{p,n} .$$

3.4. A Note on Inversion of Triangular Matrices

It may be observed that all the matrices involved in the previous sections are lower traingular. Moreover in each class, a matrix of any order is systematically connected to a matrix of next higher order. Hence the following technique for inversion of such matrices should be useful.

Let the inverse of

$$A_r = \begin{bmatrix} a_{11} & 0 & \cdots & \\ a_{21} & a_{22} & \cdots & \\ \cdot\ \cdot & \cdot\ \cdot & \cdots & \\ a_{r1} & a_{r2} & \cdots & a_{r,r} \end{bmatrix}, \tag{3.35}$$

be called A_r^{-1} . We can partition

$$A_{r+1} = \left[\begin{array}{c|c} A_r & 0_{r\times 1} \\ \hline L_r & a_{r+1,r+1} \end{array}\right], \tag{3.36}$$

where

$$L_r = (a_{r+1,1}a_{r+1,2} \cdots a_{r+1,r}) . \tag{3.37}$$

Let

$$A_{r+1}^{-1} = \begin{bmatrix} B_r & 0_{r\times 1} \\ M_r & b_{r+1,r+1} \end{bmatrix}, \tag{3.38}$$

so that

$$A_{r+1}A_{r+1}^{-1} = \begin{bmatrix} A_rB_r & 0_{r\times 1} \\ L_rB_r+a_{r+1,r+1}M_r & a_{r+1,r+1}b_{r+1,r+1} \end{bmatrix} \equiv \begin{bmatrix} I_r & 0_{r\times 1} \\ 0_{1\times r} & 1 \end{bmatrix} \tag{3.39}$$

Hence

$$(3.40)\qquad \begin{cases} A_r B_r = I_r \,, \\ \\ L_r B_r + a_{r+1,r+1} M_r = 0 \,, \\ \\ a_{r+1,r+1} b_{r+1,r+1} = 1 \,, \end{cases}$$

which gives

$$(3.41)\qquad \begin{cases} B_r = A_r^{-1} \\ \\ b_{r+1,r+1} = 1 \div a_{r+1,r+1} \,, \\ \\ M_r = -L_r A_r^{-1} \div a_{r+1,r+1} \,. \end{cases}$$

This determines A_{r+1}^{-1} from A_r^{-1}. To start with

$$(3.42)\qquad A_1^{-1} = \left[\frac{1}{a_{11}}\right] .$$

Also in all the relevent cases, L_r is known from symmetry.

To get E_{2r+1}^{-1} from E_{2r-1}^{-1}, apply the above process twice. Similarly for F_{2r+1}^{-1}.

3.5. Economisation

The conclusions derived so far regarding C_o, T_o and C_1 are valid over very short intervals of time. The technique uses the known values along Ox and at A_1 (Fig. 3.1) to yield their values for all points on A_1B_1. In the next step, A_1B_1 is taken as a new x-axis which, therefore, with the value at A_2 yields their values for all points on A_2B_2. Proceeding similarly, finally we get the values for all points on A_nB_n. Thus, provided the error does not accumulate to produce divergence, the process may be applied over a relatively larger time interval. But as suggested in section 2.1, Chapter II, the time increment $\Delta\theta$ must be kept small to avoid instability. This, however, increases the number n of time steps. To arrive at the final solution, the matrices A,B,C,E,F of order $n,n,n+1,2n+1,2n+1$ respectively are generated. This in many cases may prove to be time consuming, if not impossible, keeping in mind the limited memory space even in the largest computers. Moreover, it being a property of the Chebyshev Polynomials -- and our preference of Chebyshev polynomials over Taylor polynomials was motivated by this property -- that in a convergent series expansion of a function, the latter coefficients tend to decrease at the fastest possible rate. Thus it may happen that after a few steps, the later coefficients are less than our choice of the criterion and hence negligible for all practical purposes. It suggests that some "economisation" in the process at an intermediate stage should be

a desirable feature.

Let us suppose that for some r, the calculations yield $a_{r,r-1}$ = "zero" (i.e. less than the criterion). In obtaining the next set of coefficients, we get

$$a_{r+1,r} = \frac{\beta R^2}{16r\varepsilon_1} a_{r,r-1} \,. \tag{3.43}$$

Provided $\frac{\beta R^2}{16r\varepsilon_1} \leq 1$ (and once so, it will be true for all subsequent steps), we have

$$a_{r+1,r} = \text{"zero"}. \tag{3.44}$$

This sets up the chain process

$$a_{r+2,r+1} = \text{"zero"} = a_{r+3,r+2} = \ldots \tag{3.45}$$

Thus the $(r+1)$th step onwards significant coefficients are given by

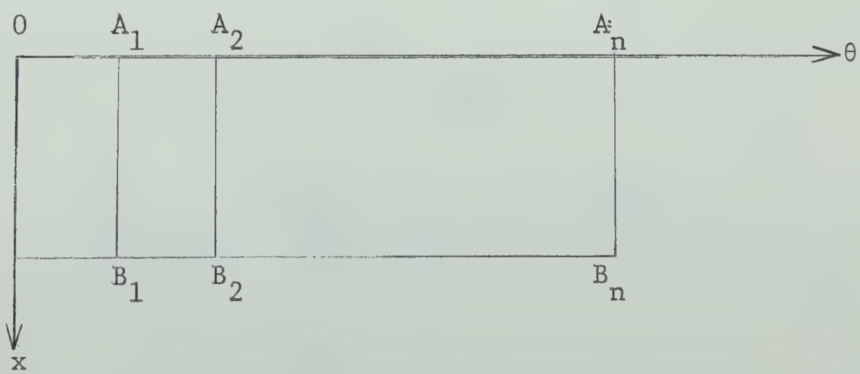

Fig. 3.1. General Scheme for the Solution of the System.

$$(3.46a)\qquad (a_{r+1,1}a_{r+1,2}\ \cdots\ a_{r+1,r-1}) = \frac{\beta R^2}{16}(a_{r,o}a_{r,1}\ \cdots\ a_{r,r-2})A_{r-1}^{-1}\ ,$$

$$(3.46b)\qquad (a_{r+2,1}a_{r+2,2}\ \cdots\ a_{r+2,r}) = \frac{\beta R^2}{16}(a_{r+1,o}a_{r+1,1}\ \cdots\ a_{r+1,r-1})A_{r}^{-1}\ ,$$

and so on. Thus the reduction of last coefficient $a_{r,r-1}$, at r*th* step, to "zero" implies that the dimension of A_r be not increased before switching to (r+1)*th* step derivation.

Now

$$(3.47a)\qquad a_{r+1,r} = \frac{\beta R^2}{16}\, a_{r,r-1} \div r\varepsilon_1\ ,$$

$$(3.47b)\qquad b_{r+1,r} = \frac{\gamma R^2}{16}\, b_{r,r-1} \div r\varepsilon_2\ ,$$

$$(3.47c)\qquad c_{r+1,r} = \frac{\lambda R^2}{16}\, a_{r+1,r} \div \xi_1\ ,$$

$$(3.47d)\qquad u_{r+1,r} = \frac{\beta R^2}{16}\, u_{r,r-1} \div r\varepsilon_1\ ,$$

$$(3.47e)\qquad v_{r+1,2r} = \frac{-\ R^2}{16\xi_2}\, \ell_{r+1,2r}\ ,$$

$$(3.47f)\qquad v_{r+1,2r-1} = \frac{-\ R^2}{16\xi_2}\left[\ell_{r+1,2r-1} - \frac{2r\varepsilon_{12}}{\xi_2}\,\ell_{r+1,2r}\right]\ ,$$

$$(3.47g)\qquad w_{r+1,2r} = \frac{-\ R^2}{16\xi_3}\, m_{r+1,2r}\ ,$$

(3.47h) $$w_{r+1,2r-1} = \frac{-R^2}{16\xi_3}\left[m_{r+1,2r-1} - \frac{4r\varepsilon_1}{\xi_3} m_{r+1,2r}\right],$$

(3.47i) $$\ell_{r+1,2r} = \frac{1}{2} a_{r+1,r} b_{r+1,r},$$

(3.47j) $$\ell_{r+1,2r-1} = \frac{1}{2}(a_{r+1,r} b_{r+1,r-1} + a_{r+1,r-1} b_{r+1,r}),$$

(3.47k) $$m_{r+1,2r} = \frac{1}{2} a_{r+1,r} c_{r+1,r},$$

(3.47ℓ) $$m_{r+1,2r-1} = \frac{1}{2}(a_{r+1,r} c_{r+1,r-1} + a_{r+1,r-1} c_{r+1,r}).$$

Hence, provided

(3.48) $$\frac{16}{R^2}(r\varepsilon_1/\beta\ ,\ r\varepsilon_2/\gamma\ ,\ \xi_1/\lambda\ ,\ \xi_2,\ \xi_3) \text{ are } \geq 1,$$

and

(3.49) $a_{r,r-1}$, $b_{r,r-1}$ and $u_{r,r-1}$ equal "zero" simultaneously

at some r<u>th</u> time step, the dimension of none of the matrices A,B,C,E and F may be increased in shifting from the r<u>th</u> step to (r+1)<u>th</u> step. In other words, after completion of each step, it will be relevent to examine if the above conditions are satisfied. If so, the dimension of none of the matrices need be raised. If not, proceed as usual.

CHAPTER IV

CONVERGENCE AND STABILITY

4.1. General Terms

In this Chapter the Convergence and Stability properties of the partial differential equations (1.25a), (1.25b) and (1.26a) will be considered. Hence it will be appropriate to have a general view of the terms involved.

In the solution of a partial differential equation in which the dependent variable U is a function of the independent variables x and t, the partial differential equation is approximated by a difference equation or an ordinary differential equation. Let u denote the solution of the approximating difference or differential equation. If $|U-u|$, often referred to as the "discretisation error", tends to zero as the increments in independent variables tend to zero, the solution is said to be "Convergent".

However, the round-off errors may affect the calculated solution u to produce the numerical solution N of the approximating equation. This gives rise to two possibilities:

(i) The error introduced at any step may increase exponentially

over the subsequent steps. Thus even if no error is introduced at a latter step, the procedure has the tendency to magnify the error at each step. Consequently, the numerical solution N may differ exponentially from the solution u. If by proper adjustment of increments in independent variables (which places limits on the values they may assume for producing a useful solution) it is possible to avoid this type of adverse situation, the method is said to be "Partially Stable". But if this is not possible, the method is called "Inherently Unstable".

(ii) If the error introduced at any step tends to decay in subsequent steps, the method is said to be "Stable".

Thus whereas the convergence implies the decay of error $|U-u|$, the stability assures the decay of the rounding error $|u-N|$. In other words, though each affects the true solution U, they are independent of each other. A process, in which calculations are performed upto an infinite number of decimal places, or in which no round-off errors are introduced, is necessarily stable.

Convergence, in general, is more difficult to investigate as it requires knowledge of the limits on the derivatives of U which, in general, are unknown. However, it is more relevant to the solution of the differential equation. Co-existence with instability is possible under certain circumstances, but convergence is a necessary condition for the usefulness of any

scheme. In some cases the round-off errors may persist linearly thus destroying a few final decimal digits, yet giving a correct solution upto a few initial decimal places. In case a scheme is unstable but convergent, it is called "Weakly Unstable" as compared to the case of "Strong Unstability" which implies non-convergence as well as instability. The former is unstable in our sense for some types of differential systems whereas the latter is always catastrophic. In case of weak instability, if we are not covering too large a range or if we are keeping a few guarding digits, a useful solution can be produced. Strong instability does not hold any such promise.

In the next sections we shall discuss the convergence and stability of the solutions C_o, T_o and C_1 of partial differential equations (1.25a), (1.25b) and (1.26a) respectively.

4.2. Convergence of $C_o(x,\theta)$

The approximation (1.29a), viz.

$$(4.1) \qquad \left[\frac{\partial C_o(x,\theta)}{\partial\theta}\right]_{r+1} = \frac{C_o^{(r+1)}(x)-C_o^{(r)}(x)}{\Delta\theta} ,$$

transforms the equation (1.25a) to the form (1.30a). Thus the true solution of the approximating equation

$$(4.2) \qquad \frac{d^2 c_o^{(r+1)}}{dx^2} - \alpha c_o^{(r+1)} = -\beta c_o^{(r)} ,$$

at a depth x and at time $(r+1)\Delta\theta$ is $c_o^{(r+1)}(x) = c_o(x, r+1\cdot\Delta\theta)$ whereas the true solution of the partial differential equation (1.25a), viz.

$$(4.3) \qquad \frac{\partial^2 C_o(x, r+1\cdot\Delta\theta)}{\partial x^2} - \frac{1}{D}\frac{\partial C_o(x, r+1\cdot\Delta\theta)}{\partial\theta} - LC_o(x, r+1\cdot\Delta\theta) = 0 ,$$

is $C_o^{(r+1)}(x) = C_o(x, r+1\cdot\Delta\theta)$. If we denote the error at the depth x at time $r + 1 \cdot\Delta\theta$ by $E_{r+1}(x)$, or simply by E_{r+1}, we have

$$(4.4) \qquad E_{r+1} = C_o^{(r+1)}(x) - c_o^{(r+1)}(x) .$$

Substituting for $c_o^{(r+1)}$ in (4.2), we get

$$(4.5) \qquad \frac{d^2 C_o(x, r+1\cdot\Delta\theta)}{dx^2} - \alpha C_o(x, r+1\cdot\Delta\theta) + \beta C_o(x, r\cdot\Delta\theta)$$

$$= \frac{d^2 E_{r+1}}{dx^2} - \alpha E_{r+1} + \beta E_r .$$

For a particular r, $r\cdot\Delta\theta$ may be regarded constant and hence

$$(4.6) \qquad \frac{d^2 C_o(x, r+1\cdot\Delta\theta)}{dx^2} = \left[\frac{\partial^2 C_o(x,\theta)}{\partial x^2}\right]_{r+1} ,$$

which from (4.3)

$$= \frac{1}{D}\frac{\partial C_o(x, r+1\cdot\Delta\theta)}{\partial\theta} + LC_o(x, r+1\cdot\Delta\theta) .$$

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Therefore,

$$\text{(4.7)} \qquad \frac{d^2E_{r+1}}{dx^2} - \alpha E_{r+1} + \beta E_r = \frac{1}{D}\frac{\partial C_o(x,r+1\cdot\Delta\theta)}{\partial\theta}$$

$$- \frac{1}{D}\frac{C_o(x,r+1\cdot\Delta\theta) - C_o(x,r\cdot\Delta\theta)}{\Delta\theta}$$

$$= \frac{1}{D}\frac{\partial C_o(x,r+1\cdot\Delta\theta)}{\partial\theta} - \frac{1}{D}\frac{\partial C_o(x,r+\varepsilon'\cdot\Delta\theta)}{\partial\theta}$$

$$= \frac{\Delta\theta}{D}\frac{\partial^2 C_o(x,r+\varepsilon\cdot\Delta\theta)}{\partial\theta^2},$$

where $0 < \varepsilon < \varepsilon' < 1$.

E_r vanishes at the boundaries $x = 0$ and $x = \infty$ for all non-negative integral r. Further, since the term $\partial^2 C_o(x,r+\varepsilon\cdot\Delta\theta)/\partial\theta^2$ denotes the rate of acceleration as far as the increase in C_o in the θ-direction at a specified depth x is concerned, it is bound to be quite small and almost constant. Therefore, let

$$\text{(4.8)} \qquad \frac{\Delta\theta}{D}\frac{\partial^2 C_o(x,r+\varepsilon\cdot\Delta\theta)}{\partial\theta^2} \doteq M .$$

The error giving equation in the final form takes the shape

$$\text{(4.9)} \qquad \frac{d^2E_{r+1}}{dx^2} - \alpha E_{r+1} = M - \beta E_r ,$$

where

$$(4.10) \qquad E_r = 0 \quad \text{at} \quad x = 0 \quad \text{and} \quad x = \infty .$$

For $r = 0$, it follows from $E_o = 0$,

$$(4.11) \qquad E_1 = \frac{M}{\alpha} e^{-\sqrt{\alpha}\, x} - \frac{M}{\alpha} .$$

For $r = 1$,

$$(4.12) \qquad (\frac{d^2}{dx^2} - \alpha)E_2 = M(1 + \frac{\beta}{\alpha}) - \frac{M\beta}{\alpha} e^{-\sqrt{\alpha}\, x} ,$$

the general solution of which is

$$(4.13a) \qquad E_2 = A_2 e^{\sqrt{\alpha}\, x} + (B_2 + \frac{xM\beta}{2\alpha^{3/2}}) e^{-\sqrt{\alpha}\, x} - \frac{M}{\alpha}(1 + \frac{\beta}{\alpha}) .$$

The boundary conditions yield

$$(4.13b) \qquad A_2 = 0 ; \quad B_2 = \frac{M}{\alpha}(1 + \frac{\beta}{\alpha}) .$$

In general,

$$(4.14a) \qquad E_{r+1} = [B_{r+1} + XB_r - X^2 B_{r-1} + \ldots - (-X)^r B_1] e^{-\sqrt{\alpha}\, x}$$

$$- \frac{M}{\alpha} [1 + \frac{\beta}{\alpha} + \ldots + (\frac{\beta}{\alpha})^r] ,$$

where

(4.14b) $$X = \frac{x\beta}{2\alpha^{\frac{1}{2}}} ,$$

(4.14c) $$B_k = \frac{M}{\alpha} [1 + \frac{\beta}{\alpha} + \ldots + (\frac{\beta}{\alpha})^{k-1}] .$$

For small values of x, the first part is approximately

$$(B_{r+1}+XB_r-X^2B_{r-1})e^{-\sqrt{\alpha}\,x} .$$

For a large r, it follows from $\frac{\beta}{\alpha} < 1$, that

$$B_{r+1} \doteq B_r \doteq B_{r-1} .$$

Hence the first part vanishes for

(4.15) $$x \doteq \frac{\sqrt{\alpha}}{\beta} (\sqrt{5} + 1) \doteq 3.236 \times \sqrt{\alpha}/\beta .$$

Also M vanishes as $\Delta\theta \to 0$.

Hence, provided the increment in x direction is small and of the order (4.15), the solution converges.

4.3. Stability of $C_o(x,\theta)$

The differential equation (1.30a) may be expressed as

$$(D^2-\alpha)c_o^{(r+1)} = -\beta c_o^{(r)} , \tag{4.16}$$

where D is the operator $\frac{d}{dx}$. Thus

$$\begin{aligned}(D^2-\alpha)^r c_o^{(r)} &= (D^2-\alpha)^{r-1}(D^2-\alpha)c_o^{(r)} \\ &= (D^2-\alpha)^{r-1}(-\beta)c_o^{(r-1)} \\ &\cdots\cdots\cdots\cdots\cdots \\ &= (-\beta)^r c_o^{(o)} .\end{aligned} \tag{4.17}$$

If $\Gamma_o^{(o)}$ is the calculated value of $c_o^{(o)}$ due to round-off error $e_o^{(o)}$ thereby propagating the error $e_o^{(r)}$ in $c_o^{(r)}$, we have

$$e_o^{(r)} = \Gamma_o^{(r)} - c_o^{(r)} . \tag{4.18}$$

Also the numerical solution $\Gamma_o^{(r)}$ satisfies the differential equation

$$\frac{d^2\Gamma_o^{(r)}}{dx^2} - \alpha\Gamma_o^{(r)} = -\beta\Gamma_o^{(r-1)} , \tag{4.19}$$

or as before,

$$(D^2-\alpha)^r\Gamma_o^{(r)} = (-\beta)^r\Gamma_o^{(o)} . \tag{4.20}$$

Equations (4.17) and (4.20), on subtraction, yield

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$$(D^2-\alpha)^r e_o^{(r)} = (-\beta)^r e_o^{(o)}, \tag{4.21}$$

the solution for which is

$$e_o^{(r)} = (A_o+A_1x+\ldots+A_{r-1}x^{r-1})e^{\sqrt{\alpha}\,x}$$
$$+ (B_o+B_1x+\ldots+B_{r-1}x^{r-1})e^{-\sqrt{\alpha}\,x} + (\frac{\beta}{\alpha})^r e_o^{(o)} , \tag{4.22}$$

which shows that error tends to increase exponentially for any x. In other words, the solution is unstable.

4.4. Convergence of $T_o(x,\theta)$

Here the partial differential equation (1.25b), viz.

$$\frac{\partial^2 T_o(x,r+1\cdot\Delta\theta)}{\partial x^2} - \frac{1}{\alpha_1}\frac{\partial T_o(x,r+1\cdot\Delta\theta)}{\partial\theta} + \sigma L C_o(x,r+1\cdot\Delta\theta) = 0, \tag{4.23}$$

by the approximation

$$\left[\frac{\partial T_o(x,\theta)}{\partial\theta}\right]_{r+1} = \frac{t_o(x,r+1\cdot\Delta\theta)-t_o(x,r\cdot\Delta\theta)}{\Delta\theta} , \tag{4.24}$$

is reduced to the form

$$\frac{d^2 t_o^{(r+1)}}{dx^2} - \gamma(t_o^{(r+1)}-t_o^{(r)}) + \lambda C_o^{(r+1)} = 0 , \tag{4.25}$$

where $t_o^{(r)} = t_o(x,r\cdot\Delta\theta)$.

Defining the error E_{r+1} as

$$E_{r+1} = T_o^{(r+1)} - t_o^{(r+1)} , \tag{4.26}$$

substituting in (4.25), and simplifying as in Section 4.2,

$$\frac{d^2E_{r+1}}{dx^2} - \gamma(E_{r+1}-E_r) = \frac{\Delta\theta}{\alpha_1}\frac{\partial^2T_o(x,r+\varepsilon\cdot\Delta\theta)}{\partial\theta^2} \tag{4.27}$$

$$\doteq M , (0 < \varepsilon < 1) .$$

Initial and boundary conditions on E_r are as for C_o with α and β both replaced by γ. Hence, in general,

$$E_{r+1} = [B_{r+1}+XB_r-X^2B_{r-1}+\ldots-(-X)^rB_1]e^{-\sqrt{\alpha}\,x} - \frac{M}{\gamma}(r+1) , \tag{4.28a}$$

where

$$X = x\sqrt{\gamma}/2 , \tag{4.28b}$$

$$B_k = \frac{M}{\gamma}(1+k) . \tag{4.28c}$$

Hence the first part vanishes for $x = 3.236/\sqrt{\gamma}$ whereas the second part approaches zero in the limit as $\Delta\theta \to 0$. This establishes

the convergence of T_o .

4.5. Stability of $T_o(x,\theta)$

Let $\tau_o^{(r)}$ be the calculated value of $t_o^{(r)}$ as obtained on solving the differential equation (4.25). Therefore,

$$\frac{d^2\tau_o^{(r+1)}}{dx^2} - \gamma(\tau_o^{(r+1)}-\tau_o^{(r)}) + \lambda C_o^{(r+1)} = 0 . \tag{4.29}$$

Subtracting it from (4.25), we have the error giving equation

$$\frac{d^2 e_{r+1}}{dx^2} - \gamma(e_{r+1}-e_r) = 0 , \tag{4.30}$$

which is the same as in the case of C_o of Section 4.3 with α and β replaced by γ. Hence the solution is unstable.

4.6. Convergence of $C_1(x,\theta)$

Arguments similar to the case of C_o of Section 4.2 lead to the error equation

$$\frac{d^2E_{r+1}}{dx^2} - \alpha E_{r+1} + \beta E_r = \frac{1}{D}\,\frac{\partial C_1(x,r+1\cdot\Delta\theta)}{\partial\theta} \tag{4.31}$$

$$+ LC_1^{(r+1)} - \alpha C_1(x,r+1\cdot\Delta\theta) + \beta C_1(x,r\cdot\Delta\theta) ,$$

which, on simplification

$$\doteq \frac{\Delta\theta}{D} \frac{\partial^2 C_1(x, r+\varepsilon\cdot\Delta\theta)}{\partial\theta^2} , \quad (0 < \varepsilon < 1) ,$$

$$\doteq M .$$

Hence the solution is convergent.

4.7. Stability of $C_1(x,\theta)$

Here the true solution of the approximating equation satisfies the differential equation

$$(4.32) \qquad \frac{d^2 c_1^{(r+1)}}{dx^2} - \alpha c_1^{(r+1)} + \beta c_1^{(r)} = C_o^{(r+1)} T_o^{(r+1)} .$$

If the calculated value, due to round-off errors, of $c_1^{(r)}$ be $\Gamma_1^{(r)}$, it satisfies the equation

$$(4.33) \qquad \frac{d^2 \Gamma_1^{(r+1)}}{dx^2} - \alpha\Gamma_1^{(r+1)} + \beta\Gamma_1^{(r)} = C_o^{(r+1)} T_o^{(r+1)} .$$

Subtracting it from (4.32), we get the error equation

$$(4.34) \qquad \frac{d^2 e_1^{(r+1)}}{dx^2} - \alpha e_1^{(r+1)} = - \beta e_1^{(r)} ,$$

which is same as in case of C_o. Hence the solution is unstable.

CHAPTER V

CONCLUSIONS AND SUGGESTIONS FOR FUTURE RESEARCH

5.1. Conclusions

To test the validity of the schemes expounded in Chapters I (where the solution has been expressed as a Taylor Series), II and III (where the solution has been expressed as a Chebyshev* Series), programs GAS1, GAS2 and GAS3, recorded in Appendix B, have been written and tested on the IBM System 360/67 at the University of Alberta, Edmonton. The numerical results have been computed for absorption of Carbon Dioxide in 1M NaOH at a pressure of one atmosphere. It is believed that the realistic values of the constants involved are as follows:

$a = 7000$

$a_1 = 17.92 \times 10^{-3}$

$a_2 = 2.9 \times 10^{-5}$

$T_o = 520.^\circ F$ (Initial Temperature)

$f_r = a.a_2.r.\Delta\theta$ lb. mole/ft.^{3}

$g_r = a.r.\Delta\theta$ °F

$\ell = 4000$

$m = 177$

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$D = 2.25 \times 10^{-8}$ ft.^{3}/sec. (Mass Diffusivity)

$\Delta = 71280$ Btu/lb. mole

$b = 9.45 \times 10^{-5}$ Btu/ft. sec. °F (Thermal Conductivity)

$\rho = 62.39999905$ lb./ft.^{3} (Molal Density)

$C_\rho = 1.0$ Btu/lb. °F (Molal Specific Hest)

If time-increment $\Delta\theta = 10^{-6}$, it follows that

$$\alpha = 0.4462222 \times 10^{14},$$

$$\beta = 0.4444444 \times 10^{14},$$

$$\gamma = 0.6603175 \times 10^{12},$$

$$\lambda = 0.30171432 \times 10^{13}.$$

For the convergence of C, it is required that the distance-step size

$$\Delta x = 3.236 \sqrt{\alpha}/\beta \doteq 0.5 \times 10^{-6}.$$

But to obtain a convergent solution for T_o, the distance-step size

$$\Delta x = 3.236/\sqrt{\gamma} \doteq 0.5 \times 10^{-5},$$

which is ten times as for C. Thus, the distance-step size has to be adjusted according as the convergence of C or T is

desired. Their relative magnitudes depend upon the system under study. Thus in many cases, as in the present one, the simultaneous convergence of C and T may not be possible due to different distance step-sizes required for each. In the present case, the convergence of C was desired and it was observed that convergence with Chebyshev* Series is much faster than with Taylor Series. In the case of Taylor Series, it was required to make 3.55×10^{-1} %. correction in C_o to get a better approximation $C_o + M \times C_1$, whereas similar correction for the Chebyshev* Series was 2.36×10^{-7} %. Thus in cases where it may be incumbent to calculate C_2 or even C_3 with Taylor Series approach, the value of C_1 calculated with Chebyshev* Series approach may give equally reliable results.

The recursion relations of Chapter II involve many multiplications at each step. This has the tendency to increase the rounding error, eroding with it the relative advantages of Chebyshev* Series over Taylor Series. Hence, in practice, the method expounded in Chapter III proves to be easiest and safest. Whereas Sullivan's [23] method is applicable for only one milli-second, this method produces a convergent solution upto ten milli-seconds.

5.2. Suggestions for Future Research

The results of Chapter IV lead us to the conclusion that system (1.30), (1.45) is convergent but unstable. This requires

a great deal of delicacy in approach in dealing with the various elements of the solution. It would be desirable to evolve a strongly stable scheme so as to achieve fast and simultaneous convergence of C and T with consistent limits on the values of Δx and $\Delta\theta$. Whereas the speed of convergence may be accelerated by employing Chebyshev* Series instead of Taylor Series (if at all such a usage becomes necessary), the other objective can be achieved by trying entirely a different type of solution. Unfortunately, Lanczos τ-method and the method of finite differences are not suited to the solution of system (1.1) and (1.4). Lanzos τ-method gives the true solution as a finite series of a slightly perturbed ordinary differential equation when an approximate solution in finite series of the true differential equation is not possible. The system (1.1), (1.4) does not qualify for this method and true finite-series solutions of (1.30), (1.45) do exist. The finite-difference approach to (1.1) and (1.4) is limited by the fact that the liquid extends to infinity.

The most promising approach might, therefore, be the modification of the semi-discrete method in which an alternative to approximation-equation (1.29) is used so as to produce a set of ordinary differential equations which are stable and converge rapidly.

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APPENDIX A

STANDARD RESULTS FOR CHEBYSHEV POLYNOMIALS

In this Appendix, a few standard results for the Chebyshev* Polynomials dealing with the range [0,1] -- in Chapter I-IV and in general referred to as Chebyshev Polynomials -- have been recorded without proof.

The general Chebyshev Function is defined by the relation

$$\text{(A-1)} \qquad T_\lambda(z) = \frac{1}{2}\left[(z+\sqrt{z^2-1})^\lambda + (z-\sqrt{z^2-1})^\lambda\right] .$$

For $\lambda = n$, the n<u>th</u> Chebyshev Polynomial associated with this symbol is

$$\text{(A-2)} \qquad T_n(z) = \frac{1}{2}\left[(z+\sqrt{z^2-1})^n + (z-\sqrt{z^2-1})^n\right] .$$

Substitution $z = x$ (real) and the change $x = \cos\theta$ reduces it to the form

$$\text{(A-3)} \qquad T_n(x) = \cos n\theta \ , \quad x = \cos\theta \ , \quad (-1 \leq x \leq 1) .$$

For the range [0,1], the change of x to $2x-1$ gives the

Chebyshev* Polynomial

(A-4) $$T^*_n(x) = T_n(2x-1) = 2T^2_n(\sqrt{x}) - 1 = T_{2n}(\sqrt{x})$$

$$= \cos(n\phi) \ , \quad \phi = \cos^{-1}(2x-1) \ , \quad (0 \leq x \leq 1).$$

Hence

(A-5) $$T^*_m(x)T^*_n(x) = \frac{1}{2}[T^*_{m+n}(x)+T^*_{m-n}(x)] \ ,$$

which for $m = 1$, gives the standard recursion formula

(A-6) $$T^*_{n+1}(x) - 2(2x-1)T^*_n(x) + T^*_{n-1}(x) = 0 \ .$$

From trigonomety

(A-7) $$\begin{cases} T^*_o(x) = 1 \ , \\ T^*_1(x) = 2x-1 \ , \\ T^*_n(x) = x^n - \binom{2n}{n}x^{n-2}(1-x) + \binom{2n}{4}x^{n-x}(1-x)^2 - \ldots \end{cases}$$

The integration formulae

$$\text{(A-8)}\quad \begin{cases} \int T_o^*(x)\,dx = \frac{1}{2}\, T_1^*(x) & , \\ \int T_1^*(x)\,dx = \frac{1}{8}\,(T_2^*(x) - T_o^*(x)) & , \\ \int T_n^*(x)\,dx = \frac{1}{4}\,\left[\frac{T_{n+1}^*(x)}{n+1} - \frac{T_{n-1}^*(x)}{n-1}\right] & , \quad n \geq 2 , \end{cases}$$

interpretted as differentian formulae and used in recursion, give

$$\text{(A-9)}\quad \begin{cases} \frac{1}{2}\,\frac{T_{2n+1}^{*'}(x)}{2n+1} = 2(T_{2n}^*(x) + T_{2n-2}^*(x) + \ldots + T_2^*(x)) + 1 & , \\ \frac{1}{2}\,\frac{T_{2n}^{*'}(x)}{2n} = 2(T_{2n-1}^*(x) + T_{2n-3}^*(x) + \ldots + T_1^*(x)) & . \end{cases}$$

Also

$$\text{(A-10)}\quad x^k T_n^*(x) = 1/2^{2k-1} \cdot \sum_{i=o}^{2k} \binom{2k}{i} T_{n+k-i}^*(x) \quad ,$$

whence

$$\text{(A-11)}\quad x^k = 1/2^{2k-1} \cdot \sum_{i=o}^{2k} \binom{2k}{i} T_{k-i}^*(x) \cdot \quad .$$

The orthogonal property of Chebyshev* Polynomials is depicted by

$$\text{(A-12)}\quad \int_o^1 \frac{T_m^*(x)\,T_n^*(x)}{\sqrt{x(1-x)}}\,dx = \begin{cases} \pi & (m=n=0) \\ \pi/2 & (m=n\neq 0) \\ 0 & (m\neq n) \end{cases} \quad .$$

If a function $f(x)$ is expanded as

$$f(x) = \frac{1}{2} a_o T_o^*(x) + a_1 T_1^*(x) + \ldots + a_n T_n^*(x) \quad , \tag{A-13}$$

to evaluate it for any x in the range, the use of recurrence relation (A-6) gives

$$f(x) = \frac{1}{2} (b_o - b_2) \quad , \tag{A-14}$$

where

$$\begin{cases} b_n = a_n \; , \; b_{n-1} = a_{n-1} + 2(2x-1)a_n \quad , \\ \\ b_r = a_r + 2(2x-1)b_{r+1} - b_{r+2} \; ,(r = n-2(-1)0) \; . \end{cases} \tag{A-15}$$

For special values of x, the results are simple and direct.

$$\begin{cases} f(1) = \frac{1}{2} a_o + a_1 + a_2 + \ldots + a_n \quad , \\ f(0) = \frac{1}{2} a_o - a_1 + a_2 - \ldots \quad , \\ f(\frac{1}{2}) = \frac{1}{2} a_o - a_2 + a_4 \quad \ldots \quad . \end{cases} \tag{A-16}$$

Also integration gives

$$\int_o^x f(x)dx = \frac{1}{2} b_o T_o^* + b_1 T_1^* + \ldots + b_{n+1} T_{n+1}^* \quad , \tag{A-17}$$

where

$$\text{(A-18)}\qquad \begin{cases} b_r = \dfrac{a_{r-1} - a_{r+1}}{4r} \;, & r = 1(1)n + 1 \;, \\[2ex] a_{n+1} = a_{n+2} = 0 & , \\[2ex] \dfrac{1}{2}\, b_o = b_1 - b_2 + b_3 - \ldots + (-1)^n b_{n+1} & . \end{cases}$$

Thus

$$\text{(A-19)}\qquad \int_o^1 f(x)dx = 2(b_1+b_3+b_5+\ldots)$$

$$= (\frac{1}{2}\, a_o - \frac{1}{1.3}\, a_2 - \frac{1}{3.5}\, a_4 - \frac{1}{5.7}\, a_6 - \ldots) \quad .$$

For differentiaition of $f(x)$, if

$$\text{(A-20)}\qquad f'(x) = \frac{1}{2}\, a_o' T_o^* + a_1' T_1^* + \ldots + a_{n-1}' T_{n-1}^* \quad ,$$

and

$$\text{(A-21)}\qquad f''(x) = \frac{1}{2}\, a_o'' T_o^* + a_1'' T_1^* + \ldots + a_{n-2}'' T_{n-2}^* \quad ,$$

where primes denote differention w.r.t. x, we have

$$\text{(A-22)}\qquad a_r' = a_{r+2}' + 4(r+1)a_{r+1} = a_{r+4}' + 4(r+3)a_{r+3} + 4(r+1)a_{r+1} \quad ,$$

so that ultimately

$$a'_r = 4[(r+1)a_{r+1}+(r+3)a_{r+3}+\dots] \quad , \tag{A-23}$$

so far as the terms vanish. Similarly, for the coefficients of second derivative

$$a''_r = 16[(r+1)(r+2)a_{r+2}+2(r+2)(r+4)a_{r+4} + 3(r+3)(r+6)a_{r+6}+\dots] \quad , \tag{A-24}$$

so far as the terms vanish.

APPENDIX B

LISTINGS OF FORTRAN IV AND APL PROGRAMS

The following pages consist of source listings of the FORTRAN IV programs GAS1, GAS2, subroutine CHSMY and APL program GAS3, subprograms LTINV1, LTINV2 and CHSMPY. The subroutine CHSMPY multiplies two Chebyshev Polynomials. The subprogram LTINV1 computes A_{r+1}^{-1} from A_r^{-1} ; subprogram LTINV2 computes E_{r+1}^{-1} from E_r^{-1}. Before calling GAS3, the values of A(=a_1), A1(=a_1), A2(=a_2), TI$_o$(= initial temperature T_o), D, RHO(= ρ), CRHO(= C_ρ), K(=k), LSMAL(=ℓ), MSMAL(=m), DELTA(=Δ), OBSVS(= time steps) and DTHETA(=$\Delta\theta$) must be specified as global variables. V specifies the vector of two elements, Δx and distance-steps respectively. The output in each case are matrices C_o, $C_o + M \times C_1$ and T_o where time increases along rows and distance increases along columns.

```
C                          GAS1
C  GAS ABSORPTION WITH CHEMICAL REACTION
C  COMPUTATATION OF ALL COEFFICIENTS RB(N) ETC.
C  PREVIOUS COEFFICIENTS PB(N) ETC.
C      INOPUT DATA IS SCALED BEFORE INPUT
C
C  ****************************************
C  *BOUNDRY CONDITIONS
C  *       FR=1.0-71.5*THETA
C  *     GR=2464789*THETA
C
C  ****************************************
C
      DOUBLE PRECISION  RB(100),PB(100),RH(200),PH(200),
     1   RG(200),PG(200),RP(200),PP(200),RQ(200),PQ(200),
     2   RU(200),PU(200),RV(200),PV(200),RW(200),PW(200),
     3   FR(100),GR(100),F(100),G(100),CONO(25,25),CONO1(25,
     4 25),TEMPO(25,25), ALPHA,BETA,GAMMA,LAMBDA,ROOT,NU,A,
     5   A1,A2,D,DELTA,KC,RHO,CRHO,TO,CO,C1,LC,MC,DTHETA,X,
     6   RL,RM,PHI,PHIBAR,PEROR
      LASTR=4
      ISTEP=10
      X=4.5D-7
      DTHETA=1.0D-6
      READ(5,30) A,A1,A2,D,DELTA,KC,CRHO,RHO
      READ(5,30) TO,LC,MC
30    FORMAT(8D10.3)
      XINC=X
      NN=1
      BETA=1/(D*DTHETA)
      ALPHA=BETA+LC/D
      GAMMA=RHO*CRHO/(KC*DTHETA)
      LAMBDA=DELTA*LC/KC
      ROOT=ALPHA**0.5
      NU=GAMMA**0.5+ROOT
32    WRITE(6,33) ALPHA,BETA,GAMMA,LAMBDA,NU
33    FORMAT('1ALPHA=  ',E12.5,5X,'BETA=',E12.5,5X,'GAMMA= ',E12.5,5X,
     1  'LAMBDA=',E12.5,5X,'NU=',E12.5)
34    WRITE(6,35) DTHETA,LASTR,X,ISTEP
35    FORMAT(' DTHETA=',F10.9,'  TIME-STEPS=',I2,'  DISTANCE-STEP-SIZE
     1  ,E10.3,'  DISTANCE-STEPS=',I2)
      WRITE(6,36) A,A1,A2,D,DELTA,KC,CRHO,RHO
36    FORMAT(' A=',E14.6,' A1=',E10.3,'  A2=',E10.3,'  D=',E10.3,
     1'  DELTA=',E10.3,'KC=',E10.3,'CRHO=',E10.3,'RHO=',E10.3)
      WRITE(6,37) TO,LC,MC
37    FORMAT('0INITIAL-TEMPERATURE=',E10.3,' LSMAL=',E10.3,' MSMAL=',
     1  E10.3)
C
C COMPUTE CONCENTRATION AND TEMPERATURE AT THE SURFACE
C
```

```
      DO 40 I=1,LASTR
      GR(I)=TO+A*I*DTHETA
      FR(I)=A1+A2*GR(I)
      F(I)=FR(I)
      G(I)=GR(I)
 40   CONTINUE
      THETA=DTHETA
      M=1
      R=0.0
      M2R=1
      M2R2=1
      RB(1)=FR(M)
      RH(1)=1.0
      RG(1)=1.0
      RM=0.0-LAMBDA*FR(M)/(ALPHA-GAMMA)
      RL=GR(M)-RM
      RP(1)=RB(1)*RG(1)
      RQ(1)=RB(1)*RH(1)
      RV(1)=RL*RP(1)/(NU*NU-ALPHA)
      RW(1)=RM*RQ(1)/(3.0*ALPHA)
      RU(1)=0.0-RV(1)-RW(1)
      PH(1)=(D*PI*ALPHA)**0.5
      PHIBAR=0.0
C
C   OUTPUT
100   IF (M.EQ.1) GO TO 275
C
C  TEST FOR LASTR.  SET PB=RB ETC.,INCREMENT.
145   CONTINUE
      IF(M.EQ.LASTR) GO TO 300
      DO 150 I=1,M
      PB(I)=RB(I)
      PH(I)=RH(I)
      PG(I)=RG(I)
      PP(I)=RP(I)
      PQ(I)=RQ(I)
      PU(I)=RU(I)
150   CONTINUE
      DO 155 I=1,M2R
      PV(I)=RV(I)
      PW(I)=RW(I)
155   CONTINUE
      THETA=THETA+DTHETA
      M=M+1
      R=M-1
      M1=M-1
      M2=M-2
      M2R=2*M-1
      M2R1=2*M-2
      M2R2=2*M-3
C
```

```
C    COMPUTE  RB
      RB(M)=BETA*PB(M-1)/(2.0*R*ROOT)
      IF(M.EQ.2)  GO TO 170
      DO 160 N=2,M1
      EN=N
      RB(N)=BETA*PB(N-1)/(2.0*(EN-1.0)*ROOT)+EN*RB(N+1)/(2.0*ROOT)
160   CONTINUE
170   RB(1)=FR(M)
C
C     COMPUTE  RH
      RH(M)=1.0
      RH(M1)=2.0*(1.0-GAMMA/BETA)*R*ROOT/(ALPHA-GAMMA)+RB(M1)/RB(M)
      IF(M.EQ.2)  GO TO 190
      DO 180 N=1,M2
      EN=N
      RH(N)=0.0-(EN+1.0)*EN*RH(N+2)/(ALPHA-GAMMA)
     1    +2.0*ROOT*EN*RH(N+1)/(ALPHA-GAMMA)
     2    -2.0*GAMMA*ROOT*R*PH(N)/(BETA*(ALPHA-GAMMA))+RB(N)/RB(M)
180   CONTINUE
C
C     COMPUTE  RG
190   RG(M)=1.0
      IF(M.EQ.2) GO TO 210
      DO 200 N=2,M1
      EN=N
      RG(N)=R*PG(N-1)/(EN-1.0)+EN*RG(N+1)/(2.0*GAMMA**0.5)
200   CONTINUE
210   RM=0.0-LAMBDA*RB(M)/(ALPHA-GAMMA)
      RL=GAMMA**0.5*RL/(2.0*R)
      RG(1)=(GR(M)-RM*RH(1))/RL
C
C    COMPUTE RP,RQ
      DO 230 N=1,M2R
      RP(N)=0
      RQ(N)=0
      DO 220 J=1,M
      IF(J.LT.(N+1-M)) GO TO 220
      IF(J.GT.N) GO TO 220
      RP(N)= RP(N)+RB(J)*RG(N+1-J)
      RQ(N)=RQ(N)+RB(J)*RH(N+1-J)
220   CONTINUE
225   FORMAT(20X,'N=',I10,5X,'P(N)=',E12.5,5X,'Q(N)=',E12.5)
230   CONTINUE
C
C    COMPUTE RV,RW
      RV(M2R)=RL*RP(M2R)/(NU*NU-ALPHA)
      RW(M2R)=RM*RQ(M2R)/(3.0*ALPHA)
      RV(M2R1)=4.0*NU*R*RV(M2R)/(NU*NU-ALPHA)
     1     +RL*RP(M2R1)/(NU*NU-ALPHA)
      RW(M2R1)=8.0*ROOT*R*RW(M2R)/(3.0*ALPHA)
     1    +RM*RQ(M2R1)/(3.0*ALPHA)
```

```
      DO 240 N=1,M2R2
      EN=N
      RV(N)=0.0-(EN+1.0)*EN*RV(N+2)/(NU*NU-ALPHA)
     1    +2.0*NU*EN*RV(N+1)/(NU*NU-ALPHA)-BETA*PV(N)/(NU*NU-ALPHA)
     2    +RL*RP(N)/(NU*NU-ALPHA)
      RW(N)=0.0-(EN+1.0)*EN*RW(N+2)/(3.0*ALPHA)
     1    +4.0*ROOT*EN*RW(N+1)/(3.0*ALPHA)-BETA*PW(N)/(3.0*ALPHA)
     2    +RM*RQ(N)/(3.0*ALPHA)
240   CONTINUE
C
C    COMPUTE   RU
      RU(M)=BETA*PU(M-1)/(2.0*R*ROOT)
      IF(M.EQ.2)  GO TO 260
      DO 250 N=2,M1
      EN=N
      RU(N)=BETA*PU(N-1)/(2.0*(EN-1.0)*ROOT)+EN*RU(N+1)/(2.0*ROOT)
250   CONTINUE
260   RU(1)=0.0-RV(1)-RW(1)
C
C     COMPUTE  PHI,  PHIBAR
      PHI=((D*PI*(R+1.0))**0.5)*(ROOT-RB(2)/FR(M))
      PHIBAR=((D*PI*(R+1.0))**0.5)*(ROOT*RW(1)+RV(1)*GAMMA**0.5
     1     -RU(2)-RV(2)-RW(2))/FR(M)
      FACTOR=(D*PI*(R+1.0))**0.5
      TERM=ROOT-RB(2)/FR(M)
270   FORMAT(5X,'******TRACE  FACTOR , TERM = ',2F12.5)
275   CONTINUE
      BSUM=0.0
      GSUM=0.0
      HSUM=0.0
      USUM=0.0
      VSUM=0.0
      WSUM=0.0
      DO 280 I=1,M
      BSUM=BSUM+RB(I)*X**(I-1)
      HSUM=HSUM+RM    *RH(I)*X**(I-1)
      GSUM=GSUM+RL    *RG(I)*X**(I-1)
      USUM=USUM+RU(I)*X**(I-1)
280   CONTINUE
      DO 290 I=1,M2R
      VSUM=VSUM+RV(I)*X**(I-1)
      WSUM=WSUM+RW(I)*X**(I-1)
290   CONTINUE
      CO=BSUM*DEXP(0.0-ROOT*X)
      TO=GSUM*DEXP(0.0-GAMMA**0.5*X)+HSUM*DEXP(0.0-ROOT*X)
      C1=USUM*DEXP(0.0-ROOT*X)+VSUM*DEXP(0.0-NU*X)
     1    +WSUM*DEXP(0.0-2*ROOT*X)
      CONO(NN,M)=CO
      CONO1(NN,M)=CO+(MC/D)*C1
      TEMPO(NN,M)=TO
      FR(M)=CO
```

```
      CR(M)=TO
      IF (M.EQ.1) GO TO 145
      GO TO 100
300   NN=NN+1
      IF(NN.LE.ISTEP) GO TO 40
      PEROR=1.0D2*( CONO1(ISTEP,LASTR) CONO(ISTEP,LASTR))/
     1   CONO(ISTEP,LASTR)
      WRITE(6,500) PEROR
500   FORMAT('0 PERCENTAGE-ERROR= ',D25.15)
      WRITE(6,127)
127   FORMAT('1****  CO  ****')
      WRITE(6,126) (F(I),I=1,LASTR)
126   FORMAT(' SURF',4(1X,D25.15))
      DO 310 I=1,ISTEP
310   WRITE(6,123)I,(CONO(I,J),J=1,LASTR)
123   FORMAT(' M=',I2,4(1X,D25.15))
      WRITE(6,128)
128   FORMAT('1****  CO+M*C1  ****')
      WRITE(6,126) (F(I),I=1,LASTR)
      DO 340 I=1,ISTEP
340   WRITE(6,123) I,(CONO1(I,J),J=1,LASTR)
      WRITE(6,124)
124   FORMAT('1***************    TO    *****************************')
      WRITE(6,126) (G(I),I=1,LASTR)
      DO 320 I=1,ISTEP
320   WRITE(6,123) I,(TEMPO(I,J),J=1,LASTR)
      STOP
      END
```

```
C                         GAS2
C
C  PROGRAM TO CALCULATE THE CONCENTRATION OF GAS AT ANY DEPTH  'R'
C
C  CONSTANTS USED ARE AS FOLLOWS * * * * *
C  DELTA  ( MEASURED IN B.T.U. PER LB. MOLE )
C  RHO : MOLAR DENSITY
C  CRHO : MOLAR SPECIFIC HEAT
C   K : THERMAL DENSITY
C   TZERO : INITIAL TEMPERATURE AT THE SURFACE
C    D : MASS DIFFUSIVITY
C  TIME : TOTAL TIME OF OBSERVATION
C  LSMAL: REACTION RATE IS K(T)=L+M.T WHERE L=LSMAL
C  MSMAL : AND M=MSMAL.
C
      INTEGER     OBSVS,OBS4,OBS1,OBS21
      DOUBLE PRECISION D,ALFA1,K,DELTA,R,TIME,LSMAL,MSMAL,L,
     1   M,NU,LAMDA,CO,TO,C1,ASUM,BSUM,CSUM,USUM,VSUM,WSUM,
     2   SALFA,SGAMA,NU,P,PEROR,AR(100),BR(100),CR(100),
     3   AR1(100),BR1(100),CR1(100),UR(100),VR(200),WR(200),
     4   UR1(100),VR1(200),WR1(200),LR1(200),MR1(200),F(100),
     5   G(100),FF(100),GG(100),CONO(25,25),TEMPO(25,25),
     6   CONO1(25,25),TO,A,A1,A2,RHO,CRHO
      DOUBLE PRECISION CON1(25,25)
1     FORMAT(8D10.3)
      READ(5,1)A,A1,A2,D,DELTA,K,CRHO,RHO
      READ(5,1)TO,LSMAL,MSMAL
C
C  INITIALISE THE CONSTANTS
C  SPECIFY  OBSVS=TIME-STEPS AND ISTEP=DISTANCE-STEPS
C  SPECIFY R=DISTANCE STEP-SIZE, DTHET =TIME STEP-SIZE
      OBSVS=4
      ISTEP=10
      DTHET=1E-6
      R=4.5D-7
      ALFA1=K/(RHO*CRHO)
      L=LSMAL/D
      M=MSMAL/D
      BETA=1/(D*DTHET)
      ALFA=BETA+L
      GAMA=1/(ALFA1*DTHET)
      LAMDA=DELTA*LSMAL/K
      SALFA=SQRT(ALFA)
      SGAMA=SQRT(GAMA)
      DSFG=SALFA-SGAMA
      NU=SALFA+SGAMA
      WRITE(6,2)  ALFA,BETA,GAMA,LAMDA,NU
2     FORMAT('   ALFA= ',D12.6,'  BETA=  ',D12.6,'  GAMA=  ',
     1   D12.6,'  LAMDA=',D12.6,'  NU=',D12.6)
      WRITE(6,3)   DTHET,OBSVS,R,ISTEP
```

```
3      FORMAT(' DELTA-THETA= ',D12.7,' TIME-STEPS= ',I5,
     1   '  DELTA-X=',D12.7,'  DISTANCE-STEPS=',I5)
       WRITE(6,4)    A,A1,A2,D,DELTA,K
4      FORMAT(' A=',D15.5 ,'  A1=',D15.5 ,'  A2=',D15.5 ,'  D='
     1   ,D15.5,'  DELTA=',D15.5,'  K=',D15.5)
       WRITE(6,5)    CRHO,RHO,LSMAL,MSMAL,TO
5      FORMAT(' CRHO=',D15.5 ,'  RHO=',D15.5 ,'  LSMAL=',D15.5
     1   ,'  MSMAL=',D15.5,'  TO=',D15.5)
       OBS4=OBSVS+4
       DO 10 N=1,OBS4
       AR(N)=0.0
       BR(N)=0.0
       CR(N)=0.0
       UR(N)=0.0
       AR1(N)=0.0
       BR1(N)=0.0
       CR1(N)=0.0
       UR1(N)=0.0
10     CONTINUE
       OBS21=2*OBSVS+3
       DO      11  N = 1 , OBS21
       VR(N)=0.0
       WR(N)=0.0
       VR1(N)=0.0
       WR1(N)=0.0
       LR1(N)=0.0
       MR1(N)=0.0
11     CONTINUE
C START CALCULATIONS FOR ONE STEP IN 'TIME' DIRECTION
       NN=1
       DO     12 I=1,OBSVS
       G(I)=TO+A*I*DTHET
       F(I)=A1+A2*G(I)
       FF(I)=F(I)
       GG(I)=G(I)
12     CONTINUE
       AR(1)=2.0    *F(1)
       CR(1) =  -2*LAMDA*F(1)/(ALFA - GAMA)
       BR(1)=2.0* G(1)-CR(1)
       VR(1) =  F(1)*BR(1)/(NU*NU-ALFA)
       WR(1) =  F(1)*CR(1)/(3.0*ALFA)
       UR(1)=-(VR(1)+WR(1))
       CO=AR(1)/2.0*DEXP(0.0-R*SALFA)
       TO=BR(1)/2.0*DEXP(0.0-R*SGAMA)+CR(1)/2.0*DEXP(0.0-R*NU)
       C1=UR(1)/2.0*DEXP(0.0-R*SALFA)+VR(1)/2.0*DEXP(0.0-R*NU)
     1   +WR(1)/2.0    *DEXP(0.0-2.0*R*SALFA)
       CONO(NN,1)=CO
       TEMPO(NN,1)=TO
       CONO1(NN,1)=CO+(MSMAL/D)*C1
       F(1)=CO
       G(1)=TO
```

```
      I=2
20    CONTINUE
      DO      22   J = 2 , I
      N=I+2-J
      AR1(N)=AR1(N+2) + (2*N/(R*SALFA))*AR1(N+1) + (R*BETA/
     1  (8*SALFA))*((AR(N-1)-AR(N+1))/(N-1)-(AR(N+1)-AR(N+3))/(N+1))
22    CONTINUE
      AR1(1)=0.0D0
      DO      24  N = 2,I
      P=(-1.0D00)**N
      AR1(1)=AR1(1)+AR1(N)*P
24    CONTINUE
      AR1(1)=2.0    *(F(I)+AR1(1))
      DO      28  J = 2 , I
         DO  28  J = 2 , I
      N=I+2-J
      BR1(N)=BR1(N+2)+2*N*BR1(N+1)/(R*SGAMA)+R*SGAMA*((BR(N-1)
     C     -BR(N+1))/(N-1)-(BR(N+1)-BR(N+3))/(N+1))/8.0
28    CONTINUE
      DO 30 J=1,I
      N=I+1-J
      CR1(N)=8*N*SALFA/(R*(ALFA-GAMA))*(CR1(N+1)-CR1(N+3))+
     1  CR1(N+2)*(1+16*N*(N+1)/(R*R*(ALFA-GAMA)))+(N/(N+2))*
     2  (CR1(N+2)-CR1(N+4))-(GAMA/(ALFA-GAMA))*((CR(N)-CR
     3  (N+2))-(N/(N+2))*(CR(N+2)-CR(N+4)))-(LAMDA/(ALFA-GAMA))
     4  *((AR1(N)-AR1(N+2))-(N/(N+2))*(AR1(N+2)-AR1(N+4)))
30    CONTINUE
      BR1(1)=0.0
      DO 32 N=2,I
      P=(-1.0D00)**N
      BR1(1)=BR1(1) + (BR1(N)+CR1(N))*P
32    CONTINUE
      BR1(1)=2.0    *(G(I)+BR1(1))-CR1(1)
      CALL  CHSMY      (I,AR1,I,BR1,LR1)
      CALL  CHSMY      (I,AR1,I,CR1,MR1)
      I21=2*I-1
      DO 38 J=2,I
      N=I+2-J
      UR1(N)=2*N*UR1(N+1)/(R*SALFA) + UR1(N+2) + (BETA*R/(8*
     1  SALFA))*((UR(N-1)-UR(N+1))/(N-1)-(UR(N+1)-UR(N+3))/
     2  (N+1))
38    CONTINUE
      DO      40 J=1,I21
      N=2*I-J
      VR1(N)=VR1(N+2)*(1-16*N*(N+1)/(R*R*SGAMA*(NU+SALFA)))+
     1   (8*N*NU/(R*SGAMA*(NU+SALFA)))*(VR1(N+1)-VR1(N+3))+
     2   (N/(N+2))*(VR1(N+2)-VR1(N+4))-(BETA/(SGAMA*(NU+SALFA
     3   )))*((VR(N)-VR(N+2))-(N/(N+2))*(VR(N+2)-VR(N+4)))+
     4   ((LR1(N)-LR1(N+2))-(N/(N+2))*(LR1(N+2)-LR1(N+4)))/
     5   (SGAMA*(NU+SALFA))
      WR1(N)=WR1(N+2)*(1-16*N*(N+1)/(3*R*R*ALFA)) + (16*N/
```

```
     1     (3*R*SALFA))*(WR1(N+1)-WR1(N+3))+(N/(N+2))*(WR1(N+2
     2     )-WR1(N+4))-(BETA/(3*ALFA))*((WR(N)-WR(N+2))-(N/(N+2
     3     ))*(WR(N+2)-WR(N+4)))+((MR1(N)-MR1(N+2))-(N/(N+2))*
     4     (MR1(N+2)-MR1(N+4)))/(3*ALFA)
 40   CONTINUE
      DO 42 N=2,I
      P=(-1.0000)**N
      UR1(1)=UR1(1)+UR1(N)*P
 42   CONTINUE
      DO 44 N=2,I21
      P=(-1.0000)**N
      VWR1=VWR1+(VR1(N)+WR1(N))*P
 44   CONTINUE
      UR1(1)=2.0   *(UR1(1) + VWR1)
      DO 46 N=1,I
      AR(N)=AR1(N)
      BR(N)=BR1(N)
      CR(N)=CR1(N)
      UR(N)=UR1(N)
 46   CONTINUE
      DO 48 N=1,I21
      VR(N)=VR1(N)
      WR(N)=WR1(N)
 48   CONTINUE
      ASUM=AR1(1)/2.0
      BSUM=BR1(1)/2.0
      CSUM=CR1(1)/2.0
      USUM=UR1(1)/2.0
      VSUM=VR1(1)/2.0
      WSUM=WR1(1)/2.0
      DO 50 J=2,I
      ASUM=ASUM+AR(J)
      BSUM=BSUM+BR(J)
      CSUM=CSUM+CR(J)
      USUM=USUM+UR(J)
 50   CONTINUE
      CO=ASUM*DEXP(-R*SALFA)
      TO=BSUM*DEXP(-R*SGAMA)+CSUM*DEXP(-R*SALFA)
      DO 52 N=2,I21
      VSUM=VSUM+VR1(J)
      WSUM=WSUM+WR1(J)
 52   CONTINUE
      C1=USUM*DEXP(-R*SALFA)+VSUM*DEXP(-R*NU)+WSUM*DEXP(-2.0*
     1   R*SALFA)
      CONO(NN,I)=CO
      TEMPO(NN,I)=TO
      CONO1(NN,I)=CO+(MSMAL/D)*C1
      F(I)=CONO(NN,I)
      G(I)=TO
      I=I+1
      IF(I.LE.OBSVS) GO TO 20
```

```
100   CONTINUE
      NN=NN+1
      IF (NN.LE.ISTEP) GO TO 12
      PEROR=1.0D2*(MSMAL/D)*CON1(ISTEP,OBSVS)/CONO(ISTEP,OBSVS)
      WRITE(6,6) PEROR
6     FORMAT('0  PERCENTAGE-ERROR= ',D25.15)
      WRITE(6,7)
7     FORMAT('1****  CO  ****')
      WRITE(6,15)  (FF(I),I=1,OBSVS)
      DO 54 I=1,ISTEP
54    WRITE(6,8) I,(CONO(I,J),J=1,OBSVS)
8     FORMAT(' XSTEP=',I2,4(1X,D25.15))
      WRITE(6,9)
9     FORMAT('1****  TO  ****')
      WRITE(6, 15) (GG(I),I=1,OBSVS)
15    FORMAT(' SURFACE ',4(1X,D25.15))
      DO 56 I=1,ISTEP
56    WRITE(6,8  ) I,(TEMPO(I,J),J=1,OBSVS)
      WRITE(6,16)
16    FORMAT('1****  CO+(MSMAL/D)*C1  ****')
      DO 60 I=1,ISTEP
60    WRITE(6, 8 ) I,(CONO1(I,J),J=1,OBSVS)
         STOP
         END
```

```
            SUBROUTINE CHSMY (M,A,N,B,W)
C
C THIS SUBROUTINE MULTIPLIES TWO SHIFTED CHEBYSHEV POLYNOMIALS
C (A0/2.T0+A1.T1+...) AND (B0/2.T0+B1.T1+...) OF DEGREES M AND N RESP.
C TO YIELD THE PRODUCT (W0/2.T0+W1.T1+...) OF DEGREE M+N
C*****INPUT=VECTORS (A0,A1,...) & (B0,B1,...)
C*****OUTPUT=VECTOR (W0,W1,...)
C
      REAL*8   A(100),B(100),W(200) ,AA(100)
      A(1)=A(1)/2.0
      B(1)=B(1)/2.0
      K=M+N-1
      DO 10 J=1,K
      W(J)=0
10    CONTINUE
      N1=1
11    DO 12 J=1,M
      AA(J)=A(J)*B(N1)
12    CONTINUE
      DO 14 I=1,M
      IN1=I+N1-1
      W(IN1)=W(IN1)+AA(I)
14    CONTINUE
      IF (M.GT.N1) GO TO 20
      DO 16 J=1,M
      I=N1-J+1
      W(I)=W(I)+AA(J)
16    CONTINUE
      N1=N1+1
      IF (N1.LE.N) GO TO 11
      GO TO 30
20    DO 22 J=1,N1
      I=N1-J+1
      W(I)=W(I)+AA(J)
22    CONTINUE
      M1=M-N1
      DO 24 J=1,M1
      J1=J+1
      N11=N1+J
      W(J1)=W(J1)+AA(N11)
24    CONTINUE
      N1=N1+1
      IF (N1.LE.N) GO TO 11
30    CONTINUE
      DO 32 I=2,K
      W(I)=W(I)/2.0
32    CONTINUE
         RETURN
           END
```

```
    ∇ GAS3 V;CON0;CON1;TEMP0;IMAR;IMBR;IMCR;IMER;IMFR;AR;
      AR1;BR;BR1;CR;CR1;UR;UR1;URX;VR;VR1;VRX;WR;WR1;WRX;F;
      FF;G;GG;I;J;N
[1]   FF←GG←F←G←OBSVSρ0×I←J←N←1
[2]   GAS31:GG[I]←G[I]←TI0+A×I×DTHETA
[3]   FF[I]←F[I]←A2×A×I×DTHETA
[4]   →((I←I+1)≤OBSVS)/GAS31
[5]   ('A=';A;' A2=';A2;' A×A2=';A×A2;' D=';D;' K=';K;' DEL
      TA=';DELTA)
[6]   ' '
[7]   ('RHO=';RHO;' CRHO=';CRHO;' LSMAL=';LSMAL;' MSMAL=';
      MSMAL;' T0=';TI0)
[8]   ' '
[9]   ('ALPHA                ';ALFA←(LSMAL+1÷DTHETA)÷D)
[10]  ('BETA                 ';BETA←1÷(D×DTHETA))
[11]  ('GAMMA                ';GAMA←RHO×CRHO÷(K×DTHETA))
[12]  ('LAMBDA               ';LAMDA←DELTA×LSMAL÷K)
[13]  ('DELTA-THETA          ';DTHETA)
[14]  ('TIME-STEPS           ';OBSVS)
[15]  ('DELTA-X              ';DX←V[1])
[16]  ('DISTANCE-STEPS       ';V[2])
[17]  ('TOTAL-TIME           ';OBSVS×DTHETA)
[18]  ('TOTAL-DISTANCE       ';V[1]×V[2])
[19]  ' '
[20]  CON0←CON1←TEMP0←(V[2],OBSVS)ρ0
[21]  IMAR←(1 1)ρ1÷EPS1←DX×(SALFA←ALFA*
      0.5)÷2
[22]  IMBR←(1 1)ρ1÷EPS2←DX×(SGAMA←GAMA*
      0.5)÷2
[23]  IMCR←(2 2)ρ(1÷XI1),0,(-EPS1÷(XI1*2)),(1÷XI1←(GAMA-
      ALFA)×(DX*2)÷16)
[24]  IMER←LTINV2(2 2)ρ(1÷XI2),0,(-(EPS1+EPS2)÷(XI2*
      2)),1÷XI2←-((GAMA+2×SALFA×SGAMA)×(DX*2)÷16)
[25]  IMFR←LTINV2(2 2)ρ(1÷XI3),0,(-2×EPS1÷(XI3*2)),(1÷XI3←-
      3×ALFA×(DX*2)÷16)
[26]  GAS32:IMAR←LTINV1 IMAR
[27]  IMBR←LTINV1 IMBR
[28]  IMCR←LTINV2 IMCR
[29]  IMER←LTINV2 LTINV2 IMER
[30]  IMFR←LTINV2 LTINV2 IMFR
[31]  →((J←J+1)<OBSVS)/GAS32
[32]  GAS33:I←J←1
[33]  AR←,2×F[I]
[34]  CR←,-LAMDA×AR÷(ALFA-GAMA)
[35]  BR←,2×G[I]-CR
[36]  VR←,BR×F[I]÷((NU←SALFA+SGAMA)*2)-ALFA
[37]  WR←,F[I]×CR÷3
[38]  UR←,-VR+WR
[39]  GAS34:CON0[N;J]←F[J]←((+/AR)-AR[1]÷2)××-DX×SALFA
[40]  TEMP0[N;J]←G[J]←(((+/BR)-BR[1]÷2)××-DX×SGAMA)+((+/CR)
      -CR[1]÷2)××-DX×SALFA
[41]  →GAS35,(URX←MSMAL×UR÷D),(VRX←MSMAL×VR÷D),(WRX←MSMAL×
      WR÷D)
```

```
[42]   GAS35:CON1[N;J]←(((-URX[1]÷2)++/URX)×*(-DX×SALFA))+((
       (-VRX[1]÷2)++/VRX)×*(-DX×NU))+(((-WRX[1]÷2)++/WRX)×*(
       -2×DX×SALFA))
[43]   →((J←J+1)>OBSVS)/GAS36
[44]   AR1←(2×F[I+1]++/AR1×Iρ 1 ¯1),AR1←AR+.×(((DX*
       2)×BETA)÷16)×IMAR[⍳I;⍳I←J-1]
[45]   BR1←BR+.×(((DX*2)×GAMA)÷16)×IMBR[⍳I;⍳I]
[46]   CR1←((GAMA×CR,0)+(LAMDA×AR1))+.×((DX*2)÷16)×IMCR[⍳1+I
       ;⍳1+I]
[47]   BR1←((2×G[I+1]++/(BR1[⍳I]+CR1[1+⍳I])×Iρ 1 ¯1)-CR1[1])
       ,BR1
[48]   PR1←(BR←BR1)CHSMPY AR←AR1
[49]   QR1←(CR←CR1)CHSMPY AR1
[50]   UR1←UR+.×(((DX*2)×BETA)÷16)×IMAR[⍳I;⍳I]
[51]   VR←VR1←((BETA×VR, 0 0)-PR1)+.×((DX*2)÷16)×IMER[⍳1+
       2×I;⍳1+2×I]
[52]   WR←WR1←((BETA×WR, 0 0)-QR1)+.×((DX*2)÷16)×IMFR[⍳1+
       2×I;⍳1+2×I]
[53]   UR←UR1←((2×++/UR×Iρ 1 ¯1)+(VR1[1]+WR1[1])-+/(VR1+WR1)
       ×2×((1+2×I)ρ 1 ¯1)),UR1
[54]   →GAS34
[55]   GAS36:→((N←N+1)≤R[2])/GAS33
[56]   ('PERCENTAGE-ERROR     ';100×|CON1[R[2];OBSVS]÷CON0[R[
       2];OBSVS])
[57]   ('****   C0   ****';FF CATC CON0)
[58]   ' '
[59]   ('****   C0+M×C1   ****';CON0+CON1)
[60]   ' '
[61]   ('****    T0    ****';GG CATC TEMP0)
[62]   ' '
       ∇
```

```
    ∇ B←LTINV1 A;N;V;I
[1]   X←÷A[1;1]
[2]   V←(I←N←1+(ρA)[1])ρ0
[3]   EX1:V[I]←N×X
[4]   →((I←I-2)>0)/EX1
[5]   I←1
[6]   EX2:V[N+1-2×I]←-I×(N-I)×N
[7]   →((I←I+1)≤⌊N÷2)/EX2
[8]   B←(A CATR(N-1)ρ0)CATC(((-V[⍳N-1])+.×A)÷V[N]),1÷V[N]
    ∇

    ∇ B←LTINV2 A;N;I;V;XI;EPS;M
[1]   V←(N←1+M←(ρA)[1])ρ0
[2]   XI←1÷V[N]←A[1;1]
[3]   EPS←-A[2;1]×XI*2
[4]   I←1
[5]   EX21:V[N+1-2×I]←M×EPS
[6]   →((I←I+1)≤⌊N÷2)/EX21
[7]   I←1
[8]   EX22:V[N-2×I]←-I×((N-1)-I)×(N-1)
[9]   →((I←I+1)≤⌊(N-1)÷2)/EX22
[10]  B←(A CATR(N-1)ρ0)CATC(((-V[⍳N-1]+.×A)×V[N]),V[N])
    ∇


    ∇ W←A CHSMPY B;I;M;N;AA
[1]   A[1]←A[1]÷2
[2]   B[1]←B[1]÷2
[3]   W←((M←ρA)+(N←ρB)-I←1)ρ0
[4]   W[¯1+I+⍳M]←W[¯1+I+⍳M]+AA←A×B[I]
[5]   →((M>I)/CHSMPY1)
[6]   W[1+I-⍳M]←W[1+I-⍳M]+AA[⍳M]
[7]   →((I←I+1)≤N)/4
[8]   →12
[9]   CHSMPY1:W[1+I-⍳I]←W[1+I-⍳I]+AA[⍳I]
[10]  W[1+⍳(M-I)]←W[1+⍳(M-I)]+AA[I+⍳M-I]
[11]  →((I←I+1)≤N)/4
[12]  W[1]←W[1]×2
[13]  W←W÷2
    ∇
```

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